FY16 NRL DoD High Performance Computing Modernization Program Annual Reports

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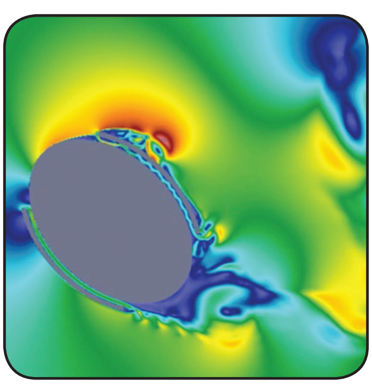
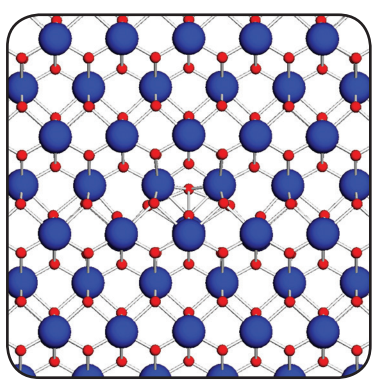
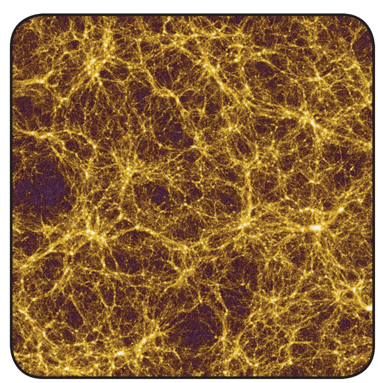

Introduction

This book is a compilation of reports on all the work accomplished by NRL scientists and engineers and their collaborators using the DoD High Performance Computing Modernization Program's (HPCMP) resources for fiscal year 2016. The reports encompass work performed by researchers at all three NRL sites: Washington, DC; Stennis Space Center, Mississippi; and Monterey, California.

These reports are categorized according to the primary Computational Technology Area (CTA) as specified by the HPCMP, and include resources at the DoD Supercomputing Resource Centers (DSRC) as well as the Affiliated Resource Centers (ARC). This volume includes three indices for ease of reference. These are an author index, a site index, and an NRL hierarchical index of reports from the Branches and Divisions in the Laboratory.

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CSM

Computational Structural Mechanics

CSM covers the high-resolution multidimensional modeling of materials and structures subjected to a broad range of loading conditions including quasistatic, dynamic, electromagnetic, shock, penetration, and blast. It also includes the highly interdisciplinary research area of materials design, where multiscale modeling from atomistic scale to macro scale is essential. CSM encompasses a wide range of engineering problems in solid mechanics, such as material or structural response to time- and history-dependent loading, large deformations, fracture propagation, shock wave propagation, isotropic and anisotropic plasticity, frequency response, and nonlinear and heterogeneous material behaviors. High performance computing for CSM addresses the accurate numerical solution of conservation equations, equations of motion, equation of states, and constitutive relationships to model simple or complex geometries and material properties, subject to external boundary conditions and loads. CSM is used for basic studies in continuum mechanics, stress analysis for engineering design studies, predicting structural and material response to impulsive loads, and modeling response of heterogeneous embedded sensors/devices. DoD application areas include conventional underwater explosion and ship response, structural acoustics, coupled field problems, space debris, propulsion systems, structural analysis, total weapon simulation, weapon systems' lethality/survivability (e.g., aircraft, ships, submarines, and tanks), theater missile defense lethality analyses, optimization techniques, and real-time, large-scale soldier- and hardware-in-the-loop ground vehicle dynamic simulation.

Title: Geometric, Constitutive, and Loading Complexities in Structural Materials
Author(s): S.A. Wimmer, A.B. Geltmacher, A.E. Moser, K. Teferra, and R.N. Saunders
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CSM

Computer Resources: SGI Altix ICE [AFRL, OH]; Cray XC40, IBM iDataPlex [ARL, MD]; Cray XE6 [ERDC, MS]

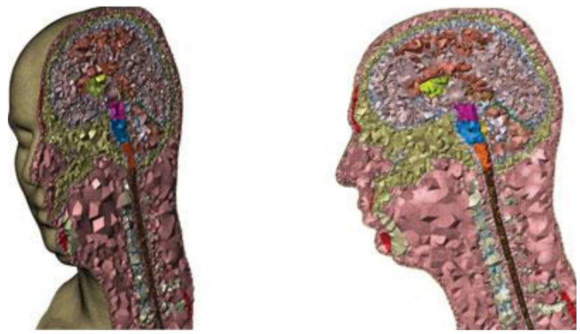
Research Objectives: The research objective is developing a rational basis and mathematical description of complex material responses for structural and novel evolving materials. Structural integrity and life cycle evaluations require an understanding of material responses. Analytical models and techniques cannot describe complex materials and often do not account for interactions, complex geometries, or multi-physics loading. Computational methods (e.g., finite elements) are used to develop models that often involve multi-functional materials, novel evolving materials, and multi-physics phenomenology. In order to accurately model the nonlinear response of conventional structural materials, rate dependence, large deformation, and damage, accumulation mechanisms must be understood and accurately represented. The performance of the overall structure or system is also examined via parameters such as kinematics, geometric complexities, loading path dependencies, and interaction between loading types.

Methodology: The project uses finite element methods extensively. Nonlinear material constitutive response features are highlighted in much of the work. Implicit and explicit solutions methods are used as appropriate. The primary finite element codes used are ABAQUS and ALE3D. User subroutines are utilized for specialized material constitutive responses when applicable. Coupled material responses, such as electrical-thermal or electrical-mechanical-thermal are exercised for evaluation of these effects. ABAQUS/Viewer, VisIt, IDL, Matlab, and Tecplot provide visualization. Model development is done with CUBIT, ABAQUS/CAE, SimpleWare, IDL, or in-house software. Large run times and large model size are often required for the multi-step nonlinear finite element analysis jobs.

Results: This project involves work in several topical areas. Work has been performed on creating image-based microstructural models, modeling multi-layer ceramic structures, biomechanics of trauma, analyses of electromagnetic launchers, modeling stress corrosion cracking, and modeling biofoulants. Representative results for one topic are presented here.

<u>Modeling of blast-induced traumatic brain injury (bTBI)</u>: Existing head models for simulating blast exposure typically have simplified geometries and inadequate material models. An improved modeling effort that overcomes these limitations is being conducted with a focus on bTBI. A high-fidelity human head model developed includes anatomically correct geometry including folds in the brain, white matter tractography (Fig. 1), and material models that describe a range of rate-dependent behaviors. It is well known that the brain fiber tracts are highly anisotropic and exist in almost all of the brain (Fig. 2). The application of an incident pressure wave (Fig. 3(a)) can greatly change the injury response in the brain when fiber tracts are accounted for (Fig. 3(b)). The injurious effect of the blast can be collected over time (Fig. 3(b)) and demonstrate the need for a computational model of the human head, which includes white matter fiber tractography. ABAQUS/Explicit is used for the analysis and typically requires 216 cores for 24 hours.

DoD Impact/Significance: TBI is one important cause of disability in the modern warfighter. Amongst the many agents in the battlefield that can cause TBI, the interaction of explosive blast with the head is the most prevalent. Thus, accurate modeling of blast-induced stress and strain waves through the head can improve our understanding of the phenomenon and aid in developing mitigation strategies and helmet designs with improved protection.



(a) (b)

Figure 1. Sagittal section of the three dimensional 3.72 million element mesh that includes linear and quadratic tetrahedral: (a) oblique view; (b) normal view.

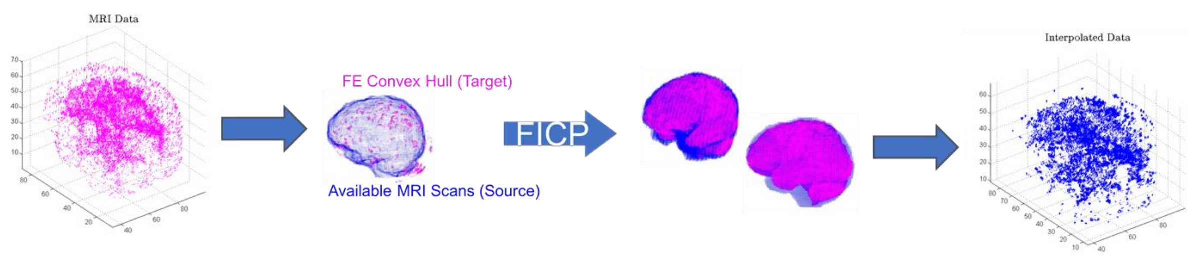
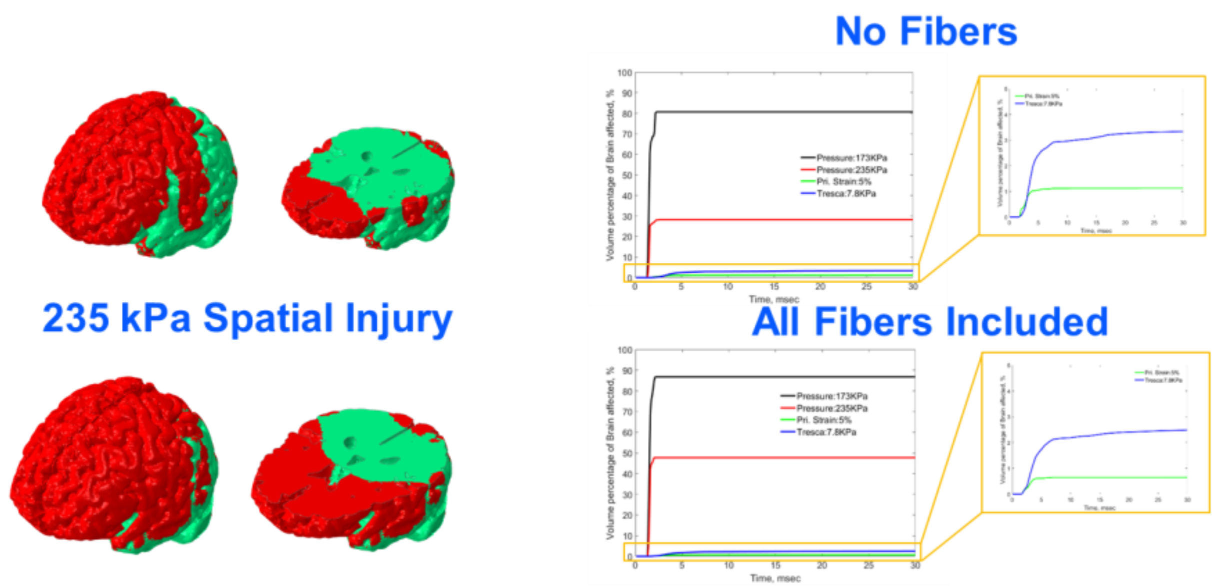


Figure 2. Transformation of MRI data of fiber tracts into the finite element space using the finite iterative closest point (FICP) method.



(a) (b)

Figure 3. The spatial (a) and temporal (b) injury results of a frontal Friedlander wave applied to the human head model. (a) The spatial injury from a 235 kPa pressure threshold in the brain with and without fibers included. The brain with fibers shows a much stiffer response and therefor more injury. The red-colored regions have experienced values beyond the respective thresholds. (b) Temporal injury generated over the entire brain volume for four criteria (173 kPa pressure, 235 kPa pressure, 5% principle strain, and 7.8 kPa shear stress). The inclusion of fiber tractography not only changes the distribution and magnitude of the injury but also the evolution of injury over time.

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CFD

Computational Fluid Dynamics

CFD covers high performance computations whose goal is the accurate numerical solution of the equations describing fluid and gas motion and the related use of digital computers in fluid dynamics research. CFD is used for basic studies of fluid dynamics for engineering design of complex flow configurations, and for predicting the interactions of chemistry with fluid flow for combustion and propulsion. It is also used to interpret and analyze experimental data and to extrapolate into regimes that are inaccessible or too costly to study. Work in the CFD CTA encompasses all velocity flow regimes and scales of interest to the DoD. Incompressible flows are generally slow (e.g., governing the dynamics of submarines, slow airplanes, pipe flows, and air circulation) while compressible flows are important at higher speeds (e.g., controlling the behavior of transonic and supersonic planes, missiles, and projectiles). Fluid dynamics itself displays some very complex physics, such as boundary-layer flows, transition to turbulence, and turbulence dynamics that require continued scientific research. CFD also must incorporate complex additional physics to deal with many real world problems. These effects include additional force fields, coupling to surface atomic physics and microphysics, changes of phase, changes of chemical composition, and interactions among multiple phases in heterogeneous flows. Examples of these physical complexities include Direct Simulation Monte Carlo and plasma simulation for atmospheric re-entry, microelectromechanical systems (MEMS), materials processing, and magnetohydrodynamics (MHD) for advanced power systems and weapons effects. CFD has no restrictions on the geometry and includes motion and deformation of solid boundaries defining the flow.

Title: Radiation MHD Modeling of High-Energy Multimaterial Z-Pinch Plasmas as a Pulsed Radiation Source*
Author(s): Y.K. Chong
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray XE6, SGI ICE X [ERDC, MS]; Cray XC40 [ARL, MD]

Research Objectives: The intense high-energy radiation and neutron sources such as the Z-pinch plasmas produced from high power pulsed generators play an important role in the support of the DoD missions such as the nuclear weapon effects study, hardness assessment analysis, and nuclear non-proliferation assays. The Z-pinch plasmas composed of different material composition and distribution offer an array of possibilities in the design, control, and optimization of the pinch dynamics, energetics and emission characteristics toward meeting the machine operation criteria. A higher thermonuclear fusion neutron yield, for example, of a deuterium double-shell gas-puff Z-pinch is predicted if the outer shell is filled with a dense high-Z gas. However, our previous RMHD study of the plasma indicates the development of multidimensional structure and non-uniform gradients as well as the complex interaction dynamics between the higher-Z outer shell material and the inner shell matter can strongly affect the radiation yield. The understanding of the complex physics and dynamical evolution of these multidimensional multimaterial plasmas is, therefore, essential in their optimal design and operation process toward meeting the mission goals.

Methodology: A multiphase multimaterial version of Machx+DDTCRE multidimensional RMHD code is applied in the study of the multimaterial Z-pinch plasma load experiments on pulsed accelerators. The material interface tracking and interaction physics control needed for the multimaterial Z-pinches are possible through a PLIC volume of fraction model. Traditionally employed approximations and adhoc models for the transport of the relevant radiation, such as the one-dimensional diffusion method due to the shear complexity in physics, and the computational limitations, are alleviated through the multiphase version of the dynamical domain tabular collisional radiative equilibrium (DDTCRE) transport models which allows a realistic description of the non-LTE ionization dynamics and radiation transport physics. An improved dynamic transport domain radiation transport model that takes advantage of the inherent compartmentalization nature of the physics will help toward efficient parallelization of the codes. The codes allow a significant freedom in the accommodation of additional details, physics, and resolution required in the proper and accurate multidimensional RMHD modeling of the plasmas produced from multimaterial element Z-pinch loads.

Results: Contrary to the idealistic 1D RMHD prediction of the thermonuclear neutron yield performance of argon outer-shell, deuterium inner-shell double-shell gas puff Z-pinch load experiments on the Sandia ZR accelerator, the 2D Machx+DDTCRE simulations study of the Z-pinch plasmas has shown that the multidimensional effects, in particular, the break-through and penetration of the argon and subsequent push-out (BP-PO) of the interior deuterium matter, significantly degrade the neutron yield performance. The study has shown that the BP-PO effects can be mitigated by having a load design that has higher linear mass density uniformity such as the Ballistic nozzle. To achieve an optimal multimaterial deuterium based Z-pinch as a pulsed neutron source via the mitigation of this adverse process, further studies in understanding the complex interaction dynamics between the outer shell material and the inner shell deuterium are needed.

DoD Impact/Significance: Insights gained through the understanding of the physics and interaction dynamics and of the complex nonlinear interaction between the non-uniform structures of multimaterial plasmas formed in different regions of hot dense multimaterial deuterium Z-pinch plasmas from the multidimensional MHD modeling study are invaluable in finding the pathway toward further improvements in their optimal design and thermonuclear neutron emission performance as a pulsed neutron source.

*This work is supported by the National Nuclear Security Administration (U.S. Department of Energy) (DOE/NNSA). Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the DOE/NNSA under contract DE-NA0001564.

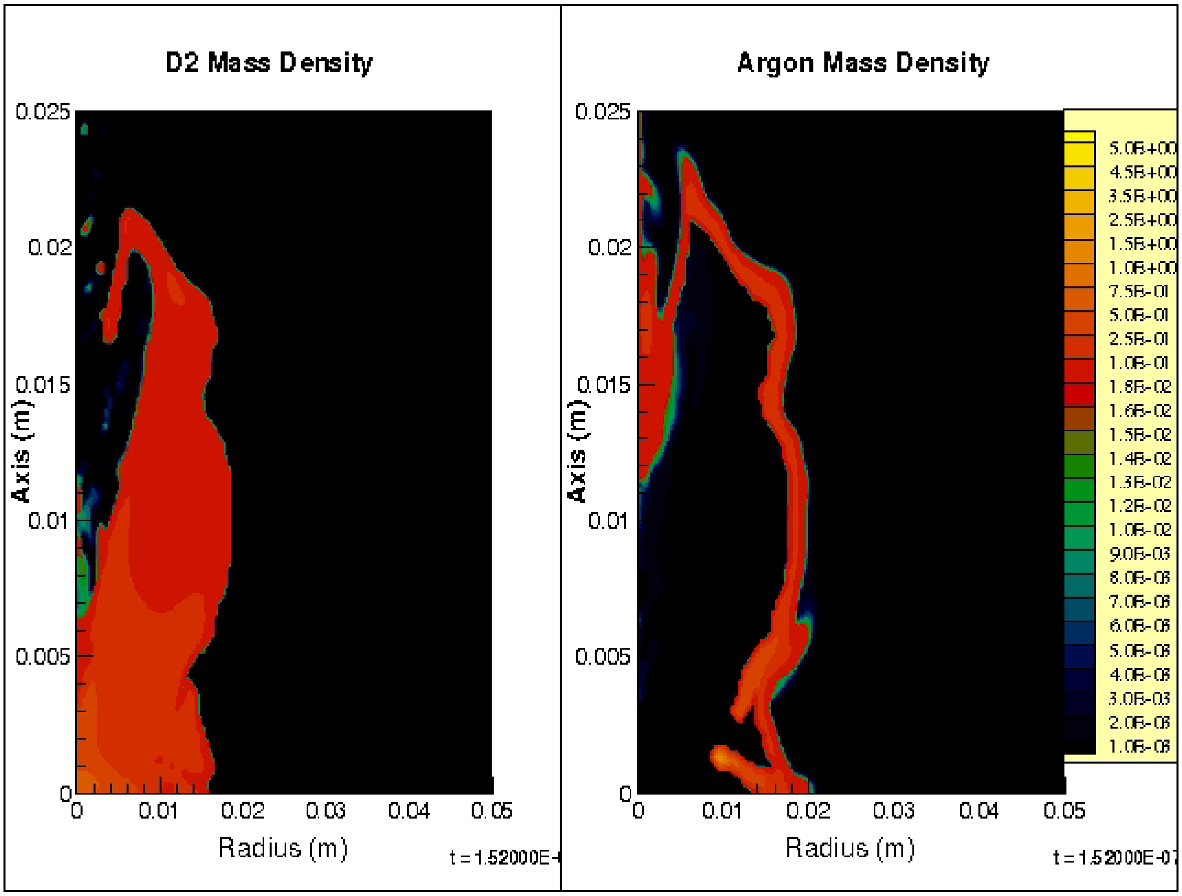


Figure 1. Color contour representation of D_2 and argon mass densities near the peak stagnation which show the break-through and penetration of the argon mass into and subsequent push-out of the interior D_2 mass as predicted from the Mach2 + DDTCRE 2D radiation MHD simulations of argon on deuterium double-shell gass puff Z-pinch load experiments on the Sandia ZR accelerator.

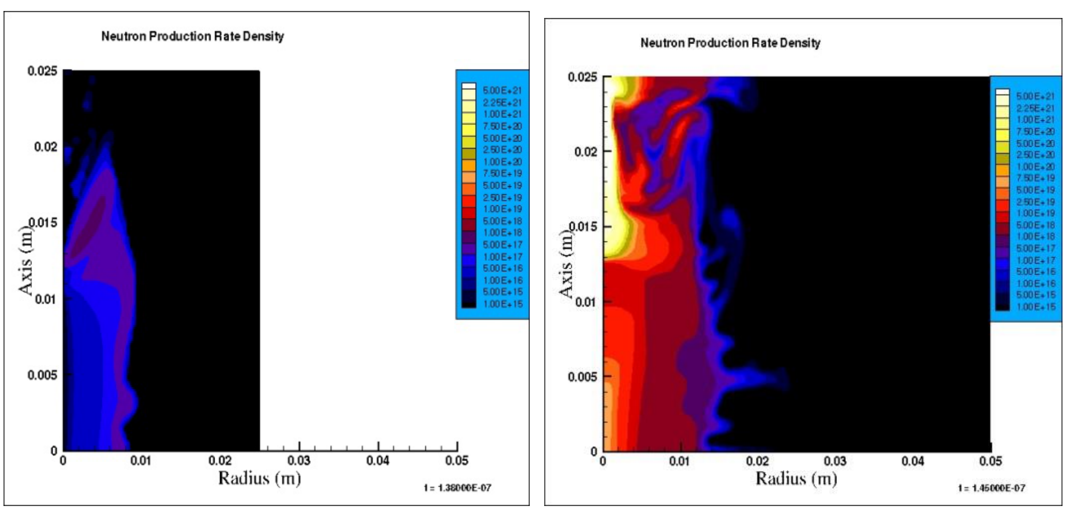


Figure 2. Color contour representation of the thermonuclear neutron production density near the peak stagnation of the argon on D_2 Z-pinch for the Alameda1234 nozzle versus the Ballistic nozzle double-shell gas puff profiles as predicted from the Mach2 + DDTCRE 2D radiation MHD simulations. The disruptive effects on the neutron yield of the argon break through for Alameda1234 nozzle is clearly evident.

Title: Numerical Simulations of Turbulence Impact on Optical Signal Transmission and Near-Surface Turbulence
Author(s): W. Hou, S. Matt, and A. Kanaev
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CFD

Computer Resources: IBM iDataPlex [NAVY, MS]; Cray XC40 [ARL, MD]; Cray XE6 [ERDC, MS]

Research Objectives: The objective of this project was to continue the work on the characterization of the Simulated Turbulence and Turbidity Environment (SiTTE). The numerical model emulates the Rayleigh-Bénard (RB) laboratory tank at NRL SSC, which allows variation of turbulence intensity. This provides the framework for repeatable experimental conditions in a controlled setting. The computational fluid dynamics model is implemented for a realistic domain size and resolves the flow down to the Kolmogorov microscale, which is required to accurately reproduce the small-scale temperature and velocity gradients affecting optical turbulence. To advance our understanding of Langmuir-type near surface coherent structures and associated turbulence, another numerical tank was set up. This tank emulates the SUSTAIN laboratory facility at the University of Miami and numerical simulations were aimed at recreating the exact experimental conditions encountered during the laboratory work.

Methodology: Very high resolution simulations were required to continue to advance the characterization of turbulence in the laboratory tank at SiTTE (Fig. 1). The experiments were implemented using the open source code OpenFOAM, in a large-eddy simulation (LES) formulation. To study near-surface turbulence in the context of Langmuir circulation, the numerical model was set up using a multiphase approach (Volume-of-Fluid) method. Wave forcing was implemented using a wave toolbox for OpenFOAM.

Results: We further explored the parameter space of the SiTTE laboratory tank and provided improved input to an optical model of beam propagation across turbulence (Fig. 2). This supports a number of projects aimed at mitigating the effects of turbulence on underwater signal transmission. We implemented a numerical model (large-eddy simulation, Volume-of-Fluid multiphase) to study Langmuir-type near-surface coherent structures and explored both wind and wave forcing in the numerical wave tank. The model uses high spatial and temporal resolution and a multi-phase formulation to capture Langmuir turbulence dynamics, without parameterizing the associated dynamics through “Craik-Leibovich” vortex force terms.

DoD Impact/Significance: The numerical simulations provide critical support for the controlled turbulence environment at SiTTE and make possible ground-breaking research and developments, such as the first remote sensing system on ocean turbulence (patent, NRL), first compressive line sensing imager with addressable illuminator (patent, NRL), first fiber optics based high speed, high accuracy temperature and flow sensor (patent, led by UNL), an innovative project to reduce boundary turbulence (DOLFIN), a project on reciprocal optical communications and the study of upper ocean processes, including air-sea interface and mixed layer dynamics, which are the basis for a proposed effort of next generation CALIPSO satellite. Advancing our understanding of the dynamics of Langmuir turbulence and associated mixing is critical for the implementation of important near-surface processes in large-scale ocean circulation and forecast models.

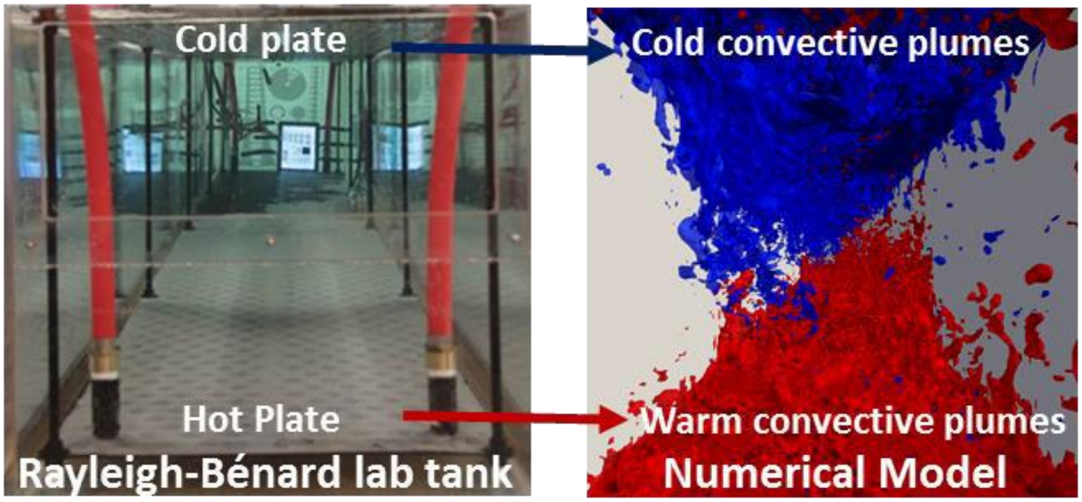


Figure 1. *Left-hand panel:* View into laboratory tank at NRL Stennis Space Center. *Right-hand panel:* Numerical model to simulate this setup.

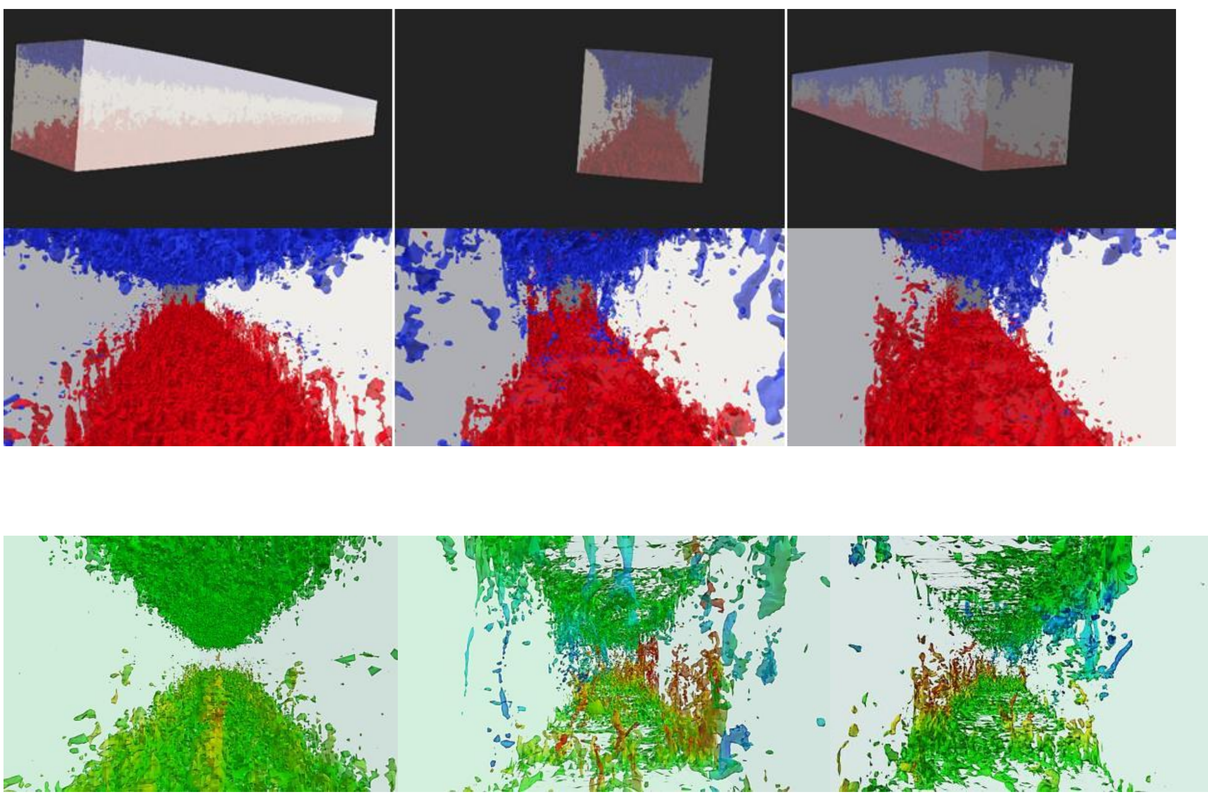


Figure 2. "Numerical Tank" used to simulate Rayleigh-Bénard convection and emulating the laboratory tank setup. *Top and middle rows*: The temperature field is shown as a fly-over around and into the tank visualizing the convective plumes as isovolumes colored by temperature range 293.6 K to 294.4 K. *Bottom row*: The same isovolumes colored by vertical velocity range -0.034 m/s to 0.0266 m/s. Frames are at model times t = 80s, 200s, 310s, top row left to right, and 70s, 330s, 880s both bottom rows, left to right.

Title: Flowfield and Transport Models for Navy Applications
Author(s): W.G. Szymczak and S. Dey
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: SGI Altix ICE [NRL, DC]; SGI ICE X [AFRL, OH]

Research Objectives: Provide resources for computational fluid dynamics simulations supporting a variety of navy applications. Examples include flow through acoustic sensors, flow and transport over passive filter shelters, and free surface flows including underwater launch and explosion bubble predictions.

Methodology: ADVED_NS is a monotone-implicit large eddy simulation code for the three dimensional incompressible Navier-Stokes equations. This code was used for predicting the peak drag force on a series of cylinders of micron diameter in a time dependent flows with fixed (acoustic) frequencies. These flows are characterized by very low Reynolds numbers on the order of 10^{-9}. These runs were performed in parallel on single cores taking advantage of the multiple processors using OpenMP, but this code is currently being modified through a PETTT project to improve scalability using the MPI based UGLIB library of routines.

Results: The ADVED_NS code was used to predict the effect of the standoff distance between micron-diameter wires and flow frequency on the total drag for an acoustic sensor. The difficulty with these simulations is the large computational domain required to eliminate boundary condition effects as well as the stiffness of the equations due to the large viscosity values. Figure 1 shows a sample computation showing flow lines and pressure contours for a flow over 3D wire mesh. Figure 2 shows verifications comparing computed and theoretical drag forces for the flow over two cylinders in an oscillating (acoustic) flow at different frequencies.

DoD Impact/Significance: The ADVED_NS runs were used to assist in the design of acoustic sensors. The results from this study demonstrated an unexpected synergistic effect in which the peak drag force and hence response of the sensor, is maximized using a specific spacing corresponding to the frequency of the acoustic flow.

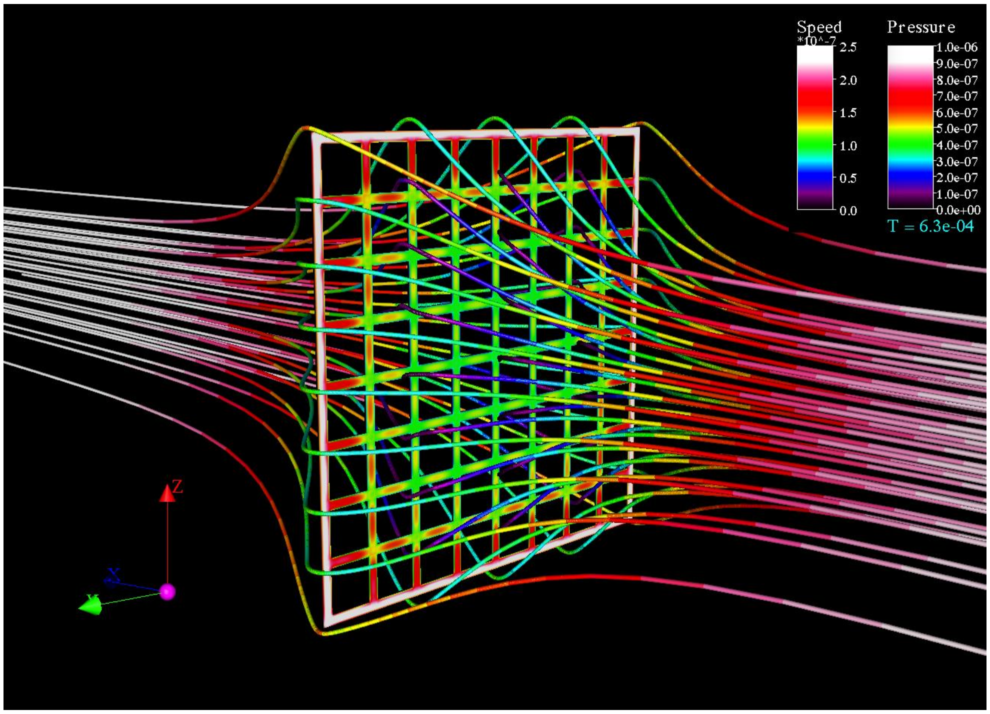


Figure 1. Pressure contours and streamlines through a 3D rectangular mesh with 20 micron spacing, Reynolds number 5.7×10^{-7}, at a frequency of 2000 Hz.

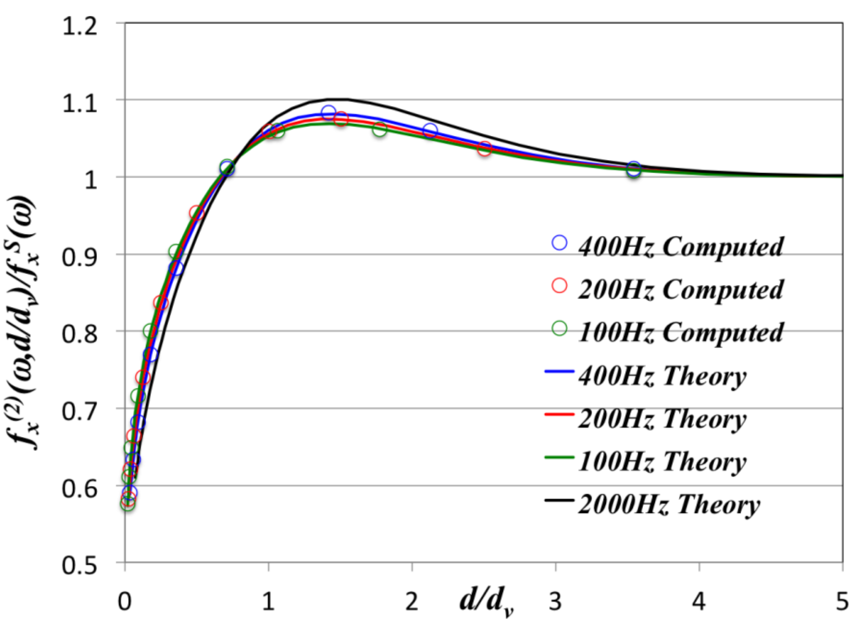


Figure 2. Peak force per cylinder for two cylinders separated by a distance *d* scaled by the viscous penetration distance $d_v = \sqrt{2\nu / \omega}$ at different frequencies. Values larger than 1 indicate a synergistic effect in which the drag per cylinder is greater than that of a single cylinder in the flow.

Title: Deflagration-to-Detonation Transition in Terrestrial Systems and Type Ia Supernovae
Author(s): A.Y. Poludnenko,[1] P.E. Hamlington,[2] C.A.Z. Towery,[2] and V.N. Gamezo[3]
Affiliation(s): [1]Texas A&M University, College Station, TX; [2]University of Colorado, Boulder, CO; [3]Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: SGI Altix ICE [NRL, DC]; SGI ICE X, Cray XC30 [AFRL, OH]; Cray XE6 [ERDC,MS]

Research Objectives: Model, understand, and predict complex reactive-flow phenomena leading to the detonation initiation in terrestrial chemical systems and thermonuclear supernovae.

Methodology: We study properties of high-speed turbulent flames by computing the interaction of a fully resolved premixed flame with a highly subsonic, statistically steady, homogeneous, isotropic turbulence. Turbulence-flame interactions are modeled using compressible reactive-flow equations solved using a fully unsplit corner transport upwind scheme with the PPM spatial reconstruction and the HLLC Riemann solver implemented in the code Athena-RFX. Turbulence is driven using a spectral method, which introduces in the flow divergence-free velocity fluctuations with a prescribed energy injection spectrum and rate. The reactive systems considered are H_2-air and CH_4-air described by one-step Arrhenius models.

Results: We consider moderate turbulent intensities corresponding to the Damköhler numbers $Da = 0.7-0.8$, and analyze the distribution of turbulent kinetic energy among different scales through the flame brush. The kinetic energy spectra shown in Fig. 1 undergo substantial changes through the flame brush from reactants to products, displaying a suppression of small-scale motions and an enhancement of the mean flow near the products. The suppression of small-scale motions is due to dilatational effects resulting from fluid expansion and the decrease in local Reynolds number resulting from the increase in viscosity with temperature. An analysis of spectral kinetic energy transfer further indicates that, contrary to the net down-scale transfer of energy found in the unburned reactants, advective processes transfer energy from small to large scales in the flame brush close to the products.

The results reveal a flux of kinetic energy that involves a cross-scale transfer through the turbulence cascade and whose prevailing direction in the flame brush is from subgrid to resolved scales. The root cause of this reversal in energy transfer, termed subgrid-scale (SGS) backscatter, is the effect of thermal expansion in the subgrid scales, by which small amounts of enthalpy created by combustion heat release are transformed into small-scale kinetic energy by means of the SGS pressure-gradient velocity correlation. The resulting overload of SGS kinetic energy is transferred to the resolved scales through SGS backscatter. This cross-scale flux of energy, along with a larger one that relies on large-scale quantities only and does not involve the energy cascade, describes the transformation of combustion heat release into kinetic energy in the turbulent premixed flame.

DoD Impact / Significance: Understanding the dynamic properties of high-speed turbulent flames provides insights for further development of turbulent combustion models for large-eddy simulations of high-speed regimes. These models are important for the theory of Type Ia supernova explosions and critical for the design of the next generation of propulsion and energy conversion systems, such as scramjet engines, rotating-detonation engines, high-pressure turbines, etc. They can also be used to predict effects of accidental gas explosions in industrial environments and help to mitigate these effects.

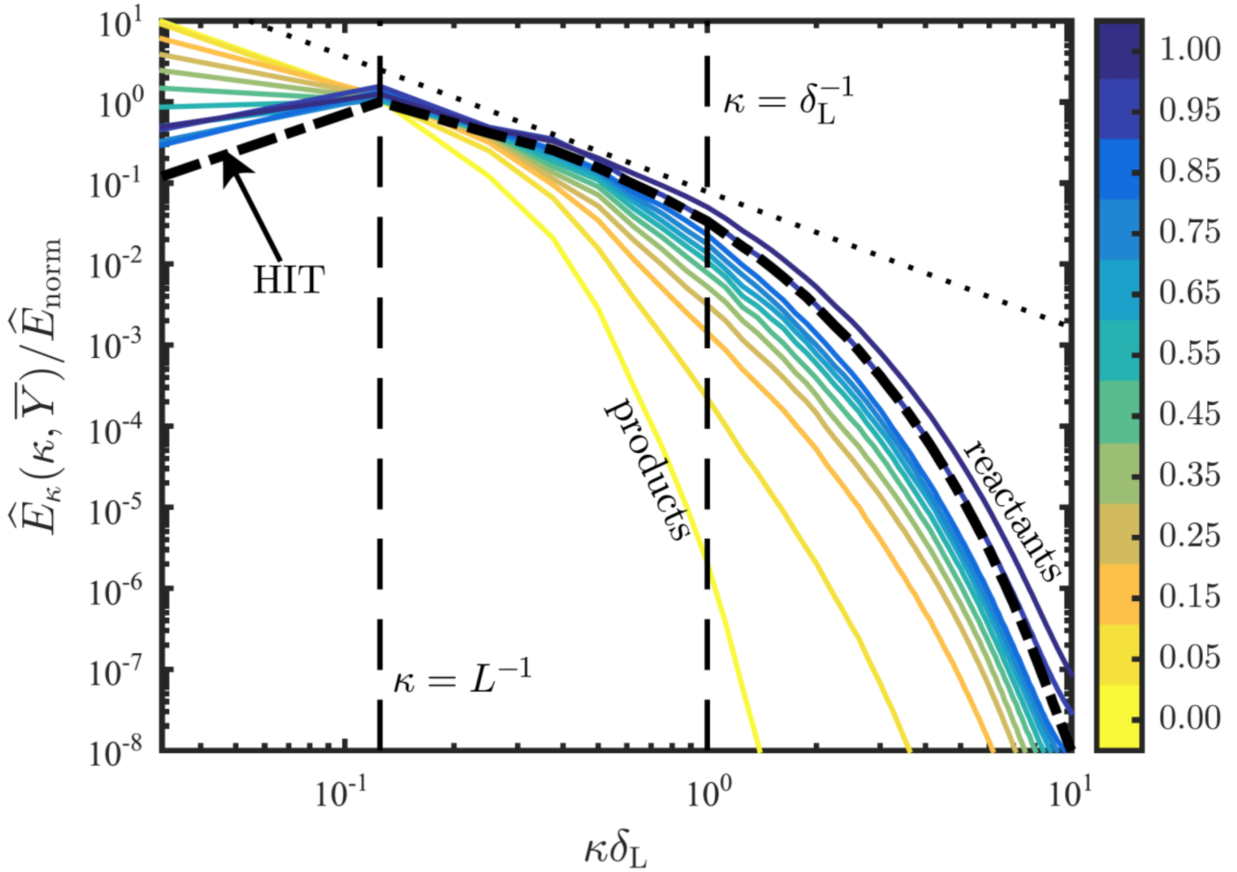


Figure 1. Isotropic turbulent spectral kinetic energy (SKE), E_κ, normalized by the forcing-scale SKE in nonreacting homogeneous isotropic turbulence (HIT) of premixed reactants, $E_{norm} \equiv E_{\kappa,HIT}(\kappa = L^{-1})$ Colored – lines correspond to various unburned mass fractions shown on color scale. Thick black line corresponds to HIT SKE. Vertical dashed lines correspond to the wave numbers of the domain width L and the laminar thermal flame width δ_L. The dotted line shows a $\kappa^{-5/3}$ spectral slope.

Title: Numerical Simulations of Noise Generated by Non-Circular Advanced Military Aircraft Nozzles
Author(s): K. Viswanath and K. Kailasanath
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

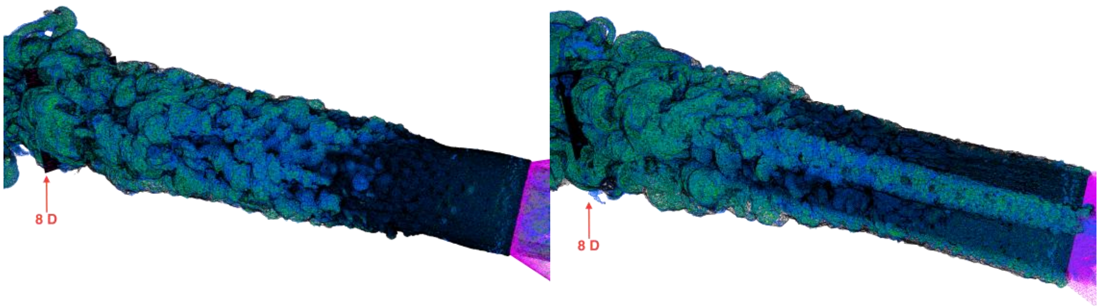
Computer Resources: Cray XC40 [ARL, MD]; Cray XE6, SGI ICE X [ERDC, MS]; SGI ICE X [AFRL, OH]

Research Objectives: To predict details of turbulent flow structures and noise generation in supersonic non-circular asymmetric exhaust jets from representative military aircraft jet engine nozzles. This information will be used to investigate and assess promising jet noise reduction concepts in support of the ongoing testing program.

Methodology: Simulations are performed using the Jet Noise Reduction (JENRE) code developed at NRL. JENRE provides unsteady compressible flow solver capabilities that support various numeric, cell-centered finite volume or nodal finite element methods, while delivering high throughput on calculations. It was developed with an emphasis on raw performance and the ability to exploit emerging massively parallel, HPC architectures including GPUs. A key bottleneck of HPC throughput is data input-output (IO). JENRE supports parallel IO via MPI/IO or the adaptable IO system (ADIOS). JENRE uses an edge-based formulation for all flux integration and limiting algorithms. Taylor-Galerkin finite element method with second order spatial accuracy, for tetrahedral cells, is used with the Finite Element Flux Corrected Transport (FEM-FCT) method. The multi-dimensional FCT flux limiter provides an implicit subgrid stress model, which ensures monotonicity at shocks and sharp gradients with minimal artificial dissipation. JENRE supports in-situ calculation of far-field noise data using the Ffowcs Williams and Hawkings (FW-H) approach using resolved nearfield data in the domain. This greatly decreases noise processing related IO and storage and outputs noise data, and the spectrum of the normalized pressure fluctuations as a spectral density field for specified locations at the farfield. With a span of such recording locations, the asymmetric nature of the non-circular nozzle noise generation can be investigated along with recording the observer orientation dependence on the noise propagation for different nozzle configurations.

Results: A rectangular nozzle, with an aspect ratio of 2, an equivalent diameter circular nozzle of the same design Mach number were simulated to provide comparison in noise production and flow features. A larger aspect ratio rectangular nozzle with configurable features such as an aft deck of variable length, single expansion ramp (SERN), and a secondary stream mixing into the main flow were also simulated to model future nozzle requirements of aircraft frame integration and flow control in collaboration with Air Force Research Lab (AFRL). The simulated acoustic data were validated against experimentally recorded sound pressure level (SPL) spectra, with very good agreement. The dynamics of the large-scale coherent structures are shown to be different between the rectangular and the circular jets, with streamwise vorticity and corner effects being a factor in the rectangular jets leading to enhanced entrainment. Phase averaged streamwise velocity and vorticity plots at various cross sectional planes and 3D iso-surfaces of Q-criterion show that there is strong self-induction and stretching of the large scale coherent azimuthal structures, especially at the corners, that differentiate the mixing features of the rectangular from the circular jet. The streamwise vorticity dynamics are affected by the variation of the self-induction of the azimuthal vortex ring around the rectangular nozzle lip. The initial vortex setup and subsequent interaction inhibited axis-switching for these rectangular jet cases. The secondary stream mixing in and the length of the aft-deck, sitting flush with bottom nozzle lip, emerged as further toggles that affected the far-field noise in the case of the larger aspect ratio nozzle.

DoD Impact/Significance: Our work will provide better understanding of the noise production for both industrial and military aircraft, and will aid the current effort of noise reduction, especially for supersonic aircrafts to reduce the impact of the jet noise on shipboard health and safety issues. Futuristic nozzles are tending towards non-circular geometries for flexibility in airframe integration, capabilities such a SERN profile, and other potential advantages.



(a) Circular (b) Rectangular

Figure 1. Dynamics of the azimuthal vortex ring for circular and rectangular jets at TR 1.0. The iso-surfaces of vorticity and qcriterion are shown till 8 D axial distance. Jet direction is from right to left.

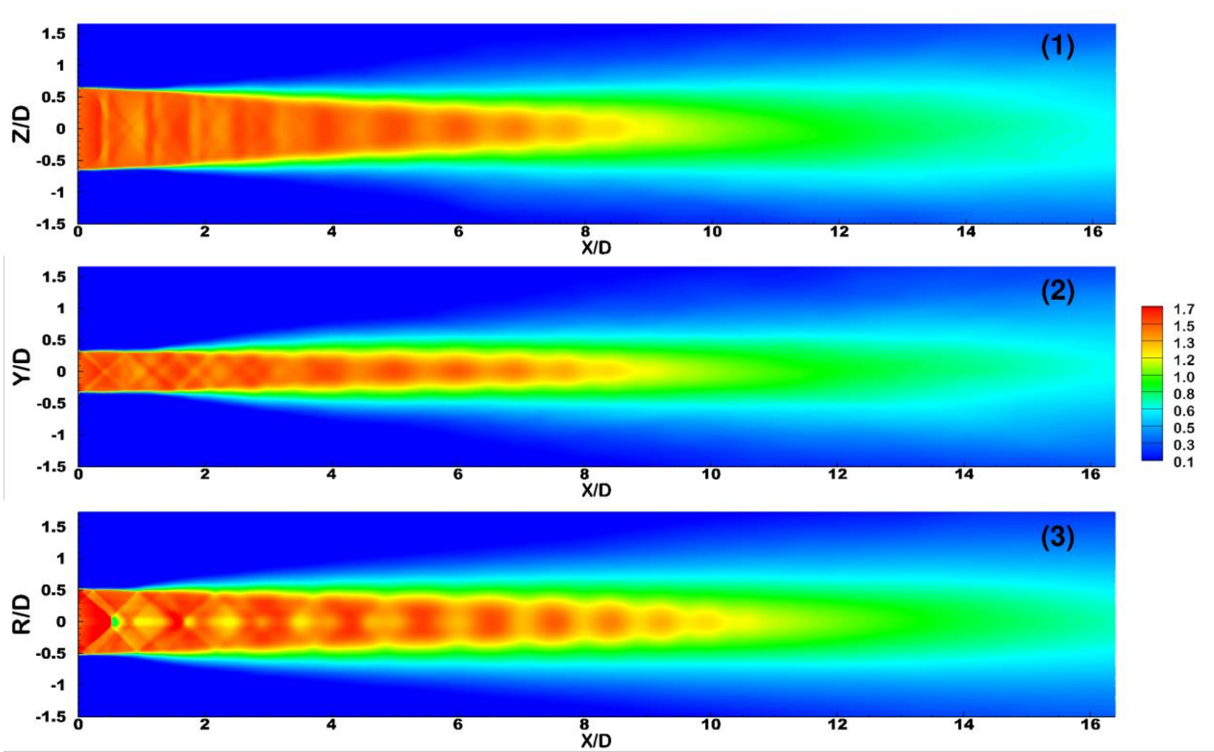


Figure 2. Time averaged velocity distributions for the heated jets, TR = 3.0. (1) Major axis plane. (2) Minor axis plane for rectangular jet. (3) Center plane from circular jet.

Title: Multidimensional Chemically Reacting Fluid Dynamics
Author(s): R. Johnson, A. Kercher, D.A. Schwer, and K. Kailasanath
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray XC30 [AFRL, OH]; Cray XC40 [ARL, MD]; Cray XE6 [ERDC, MS]

Objectives: Use the HPC computational resources to simulate the computationally expensive chemically reacting fluid dynamics in various multidimensional configurations with the goal of better understanding various complex, multi-scale, combustion phenomenon.

Methodology: The codes written under the HyCC framework and currently in use at The Laboratories for Computational Physics and Fluid Dynamics can accurately predict the flow field in many configurations. These codes employ high order methods, which are capable of simulating unsteady flows with strong shocks, chemical reactions, and other complex features. This work focuses on developments that are currently underway which will allow for the simulation of high speed and low speed reacting flows using state-of-the-art numerical methods. This year, we produced several important results, building the necessary components required to simulate reacting fluid dynamic systems.

Results: HPC resources were used extensively to study the effect of body armor on evaporative cooling for idealized torso geometries using passive species tracking throughout the simulations. For the study, one hundred and eight fluid dynamic simulations were preformed, each corresponding to a different body armor configuration. Results were used to estimate the amount of cooling provided by each armor configuration. HPC resources were also required for simulations of incompressible fluid flowing through a channel with oscillating walls. These simulations were extremely computationally extensive since they required the entire spacetime domain to be solved simultaneously. Both species transport and spacetime domain results are essential in the development process of the reacting fluid dynamics.

DoD Impact/Significance: Accurately predicting combustion has benefits to Navy engine technologies. In order to predict combustion in complex settings, we must first start with validating our prediction techniques. The research performed this year has applications to these combustion systems as each one tests the current state of the art's ability to predict a separate combustion phenomena. The information generated by the species transport study not only gave insight to our code's capability of predicting diffusion phenomena, but also gave useful results for military body armor. The spacetime geometry tested the ability of our code to solve physical systems in space and time with an all-at-once approach. This will be important for predicting military combustion systems as they interact with complex geometries (such as combustors) and recessing surfaces (such as deck ablation).

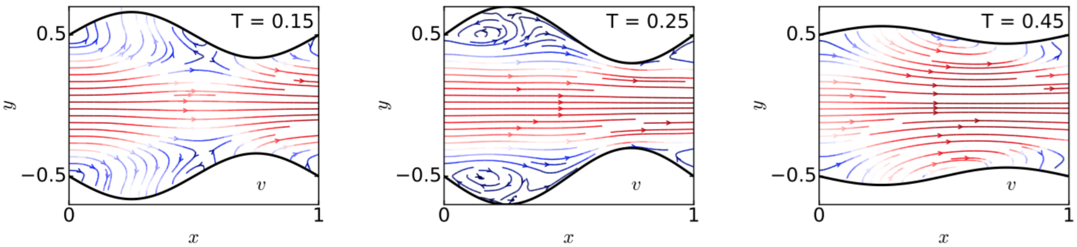


Figure 1. Spacetime simulation of incompressible flow through a channel with oscillating walls at different times, T. Simulations were performed in a three dimensional grid, where the third dimension was time.

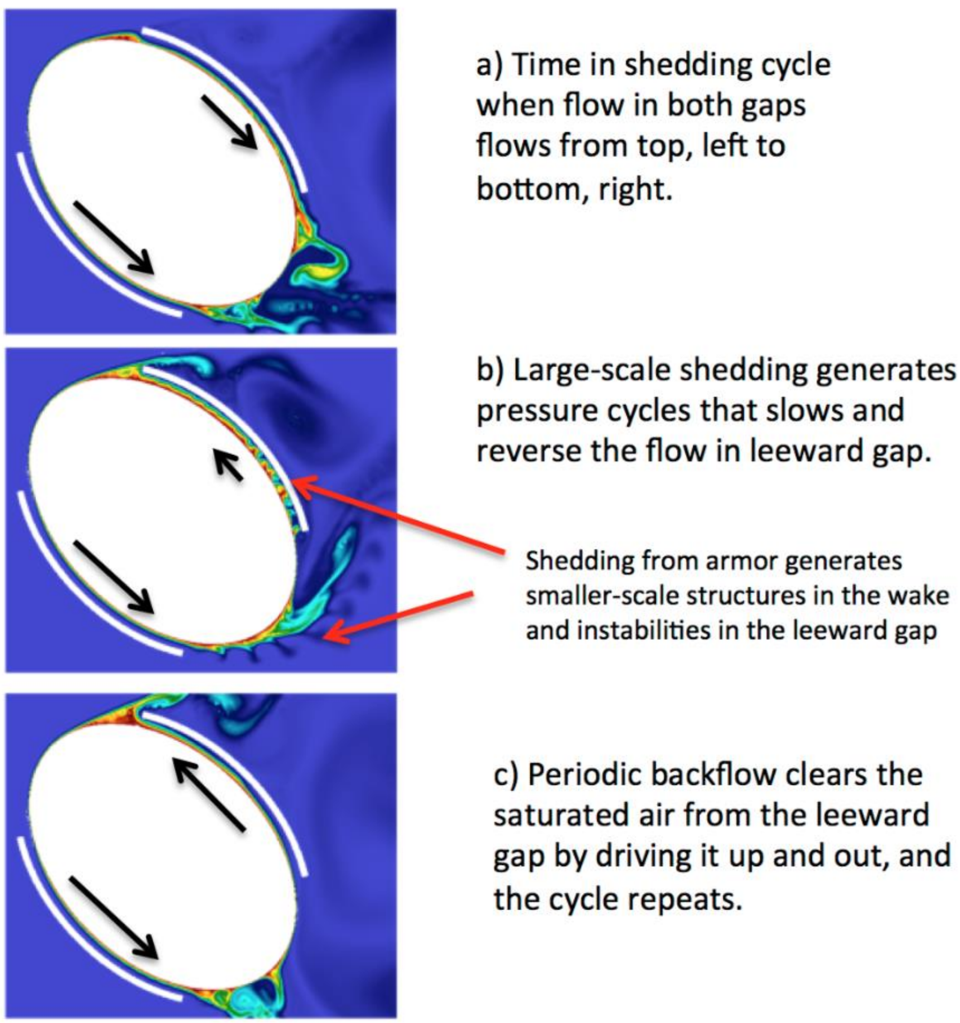


Figure 2. Simulation results of flow around body armor configuration demonstrating accurate species diffusion.

Title: Applications of FEFLO Incompressible Flow Solver
Author(s): R. Ramamurti
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: SGI Altix ICE [NRL, DC]

Research Objective: Perform three-dimensional (3-D) numerical simulations of flow past complex configurations. The proposed studies will investigate the use of bio-inspired fins for underwater propulsion as well as aerodynamic control surfaces for the development of a novel hybrid vehicle.

Methodology: A finite element solver, called FEFLO, for 3-D incompressible flows based on unstructured grids is used. The flow solver is combined with adaptive remeshing techniques for transient problems with moving grids and is also integrated with the rigid body motion in a self- consistent manner which allows the simulation of fully coupled fluid-rigid body interaction problems of arbitrary geometric complexity in three dimensions. NRL has developed a flapping fin UUV for effective low speed operations. A new hybrid UAV/UUV, called the Flimmer, is developed for long-range transit and high speed air delivery of these vehicles to near shore operational zones.

Results: For the hybrid vehicle Flimmer, the flapping fins of the UUV are used not only as underwater propulsors but also as aerodynamic control surfaces in air. Computational fluid dynamics studies of the 3-D unsteady flow past the Flimmer were conducted to address its performance during its glide phase in air, swimming underwater, and the landing phases. The swimming performance of the hybrid vehicle and the swimming-only vehicle were assessed at various vehicle velocities and kinematics of the flapping fins. At a flapping frequency of 0.35Hz and an amplitude of 148°, the hybrid vehicle with 4 flapping fins were able to produce enough thrust to propel at around 1kt. For the swimming only prototype, at a flapping frequency of 0.8Hz and an amplitude of 78°, the fins were able propel the vehicle at 1.3kts.

DoD Impact/Significance: Simulations have enabled characterization of the aerodynamic performance of the hybrid vehicle, the thrust and lift generation mechanisms in flapping foil propulsion for unmanned underwater vehicles, and the loads experienced during the water landing. This enables a new capability to assess the performance of unconventional unmanned vehicles.

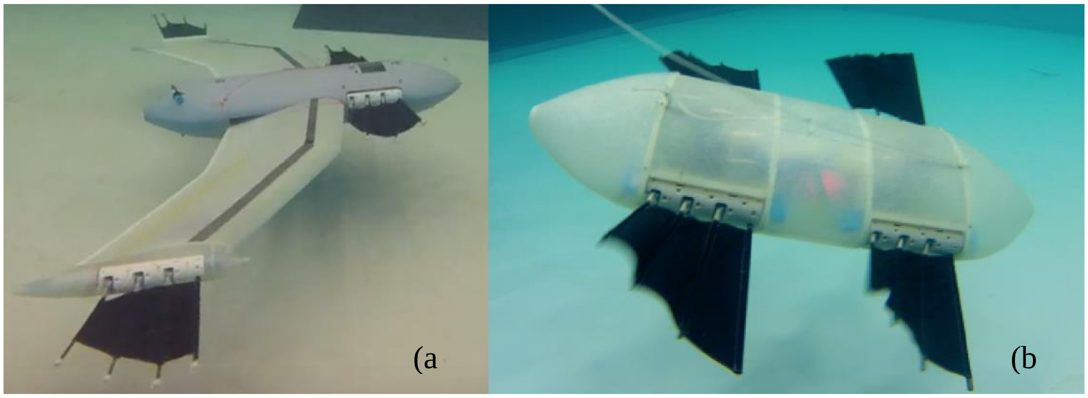


Figure 1. Flimmer prototype showing (a) hybrid vehicle with fixed wing and (b) swimming vehicle.

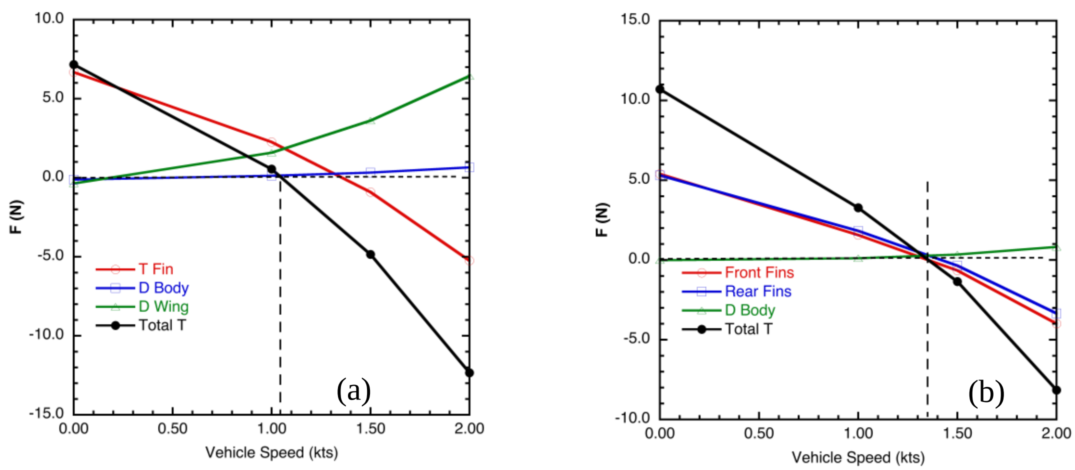


Figure 2. Performance of the Flimmer vehicle with four flapping fins, (a) hybrid vehicle at f= 0.35Hz, and (b) swimming vehicle at f = 0.8Hz.

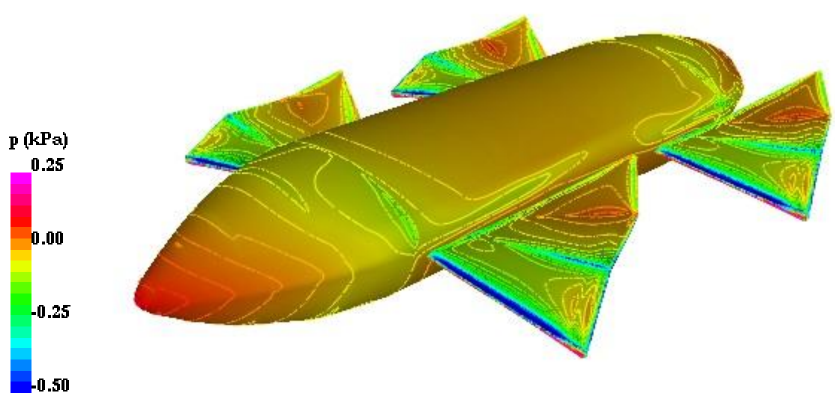


Figure 3. Surface pressure distribution over the swimming vehicle, f = 0.35Hz, V= 1kt.

Title: Fine Scale Structure of the Air-Sea Interface

Author(s): G.B. Smith,[1] R. Leighton,[2] I. Savelyev,[1] and T. Evans[1]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]SRI-International, Ann Arbor, MI

CTA: CFD

Computer Resources: SGI Altix ICE [NRL, DC]; SGI ICE X [ARFL, OH]

Research Objectives: The research objectives of this multi-year effort are to understand the coupling small-scale processes at the air-sea interface to ocean mixed layer process. Recently a primary focus has been the contribution to upper-ocean mixing due to Langmuir circulation. The genesis of Langmuir circulation is a very complex process and an area of active scientific research. Classical theory posits that these structures result from the interaction of ocean wave generated Stokes drift and the surface current due to wind shear. This process is a primary driver in the transport of mass, momentum and heat through the mixed layer, but remains a critical missing element in flux modeling at the interface. The specific research objective is to quantify the level of circulation induced surface straining and the impact of that straining on the near surface boundary layer.

Methodology: Two parallel approaches are currently being pursued in this project. In the first, the numerical simulations are performed using a well-established pseudo-spectral code that can be run in a DNS (Direct Numerical Simulations) or LES (Large-Eddy Simulation) mode. The algorithm has been extended to include the transport of thermal energy and mass, via the Boussinesq approximation and includes an explicit stokes drift term. The simulations are being benchmarked against available in-house infrared imagery of Langmuir circulation. In the second, a different code is used to simulate a smaller scale 'patch' of Langmuir turbulence. This code is also run in a DNS mode, but in this case a passive scaler has been added to the water surface. This passive scaler simulates the behavior of dye on the surface, and is being benchmarked against results from a dye release experiment conducted in October/November 2015.

Results: The primary activity in FY16 has been the comparison of flow structures observed in the infrared at the University of Delaware Air-Sea Interaction Laboratory similiar in appearance to Langmuir cells (Fig. 1). While small waves were observed in the experiments, comparisons to complementary numerical simulations indicate the observed structures are not Langmuir cells, but are most likely related to turbulent shear flow. The cross section of the temperature field for numerically simulated Langmuir cells can be seen in Fig. 2(a). The temperature is scaled using the heat flux out of the interface and the lengths are scaled using the shear stress. The descending thermal structure are driven by the downward directed Langmuir forcing, which is active (non-zero) only to a depth of 10-15 for this simulation. The vertical line in Fig. 2(b) of the surface temperature defines the location of the vertical cut. The descending cool plumes originate in the convergence zones of the Langmuir cells. Figure 3 shows early results from the second simulation with imagery from the actual dye release for comparison. The entire flow field of approximately 600 m in length could not be simulated directly, so individual 'patches' of approximately 30 m square were stitched together. While preliminary, the results compare favorably qualitatively. Work is continuing on both fronts in FY17.

DoD Impact/Significance: This activity has two potential Naval applications. The primary application is in the development of improved flux models for the air sea interface. Specifically, fully coupled air-ocean models, wherein the ocean boundary layer is not fully resolved numerically, would benefit from high-resolution interfacial flux modeling. A secondary Naval application would be the inversion of remote sensing data, specifically combined thermal infrared and visual imagery, for the evaluation of the properties of the ocean mixed layer. Although not as operationally significant as the first application, the inversion of this type of remote sensing data would have significant research utility.

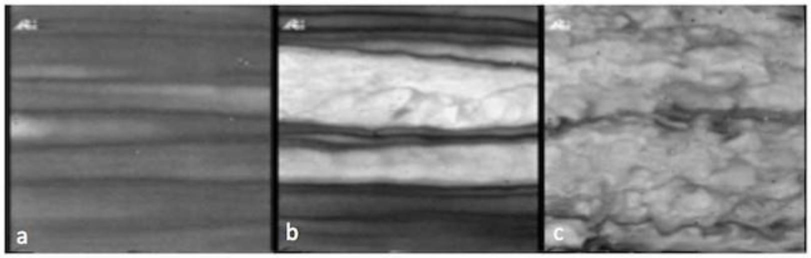


Figure 1. A sequence of infrared images showing a transition to turbulent flow. Langmuir forcing resulting from the nonlinear interaction of the wind shear and Stokes drift does not appear to be relevant for the post-transitional steady state (c), though it may have been present during the transition (b).

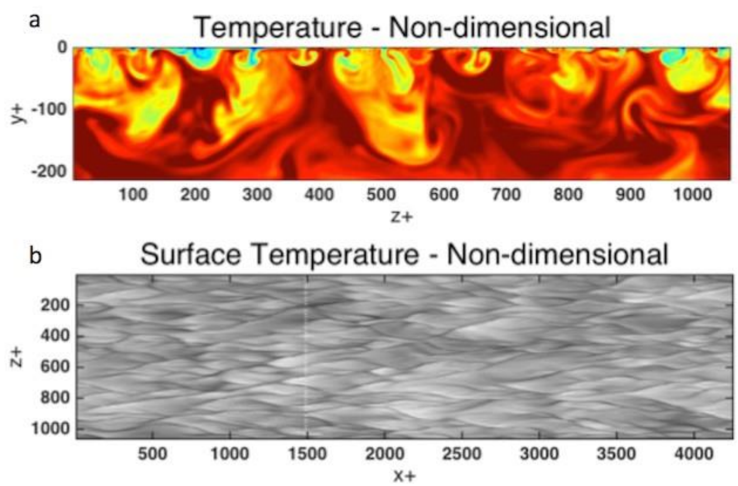


Figure 2. Temperature field from a direct numerical simulation of Langmuir cells. (a) Temperature field in a cross section showing the cool (blue-yellow) descending plume. (b) The convergence zones due to the Langmuir cells compress the thermal boundary layer and allowing locally cooler temperatures. Vertical line in (b) is the location of the cross section.

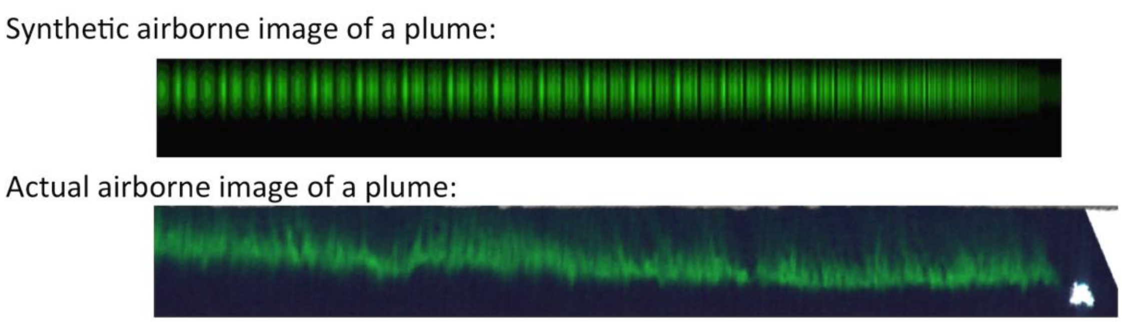


Figure 3. Comparison of results from simulated and actual dye releases. Upper frame contains a sample of simulated results. Lower frame shows airborne imagery taken of dye released from a boat as it traveled from left to right across the scene. The dye on the left edge of the image was released approximately 20 minutes before that on the right edge. Since the entire scene could not be simulated during one run the upper frame was assembled from simulation output taken from different times chosen to correspond to the times from the actual experiment. Qualitative agreement is quite good, and analysis is continuing.

Title: Simulations of Supersonic Jet Noise and Impact of Inflow Turbulence on Jet Noise of Military Jet Engines
Author(s): J. Liu, A. Corrigan, R. Ramamurti, and K. Viswanath
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: SGI ICE X [AFRL, OH], Cray XE6, SGI ICE X [ERDC, MS]; Cray XC40 [ARL, MD]

Research Objectives: The objective is to use numerical simulations to improve understanding of the mechanisms of noise generation and to develop noise reduction technique to reduce noise of the supersonic military aircraft operating at design and off-design conditions.

Methodology: Large-eddy simulations are carried out using our in-house jet noise simulation code, JENRE. It is a Navy based, NRL developed flow solver, which uses both finite volume and finite element approaches. It can take structured meshes and unstructured meshes with arbitrary cell types and has multiple levels of parallelism: Multi-core CPUs or Multi-core GPUs, and MPI for inter-processor communication. JENRE has achieved an exceptional computational performance and scalability. The far-field noise prediction tool, which uses the Ffowcs Williams & Hawkings (FW-H) Surface Integral method, has also been implemented in JENRE. To take into account the high-temperature effect observed in realistic jet engine exhausts, a temperature dependent function of the specific heat ratio is developed and is implemented in JENRE.

Results: Since temperatures of the realistic jet engine exhausts are high, it is important to understand the high-temperature effect on the jet noise generation. However, it is difficult to investigate this effect in laboratory settings because it is difficult to generate and continually supply high-temperature air, thus, large-eddy simulations are used as a preferred approach for this study. We have implemented a temperature-dependent specific heat ratio in JENRE and have compared results to those using a constant specific heat ratio. It is found that using a constant specific heat ratio will modify the nozzle-exit conditions and thus introduce some discrepancies in the prediction of the shock-associated noise. But the discrepancy in the peak noise level is small. In addition, it is found that the noise distribution is dominated by two major radiation directions in the form of a dual-lobe pattern as shown in Fig. 1. This dual-lobe pattern is similar to those observed in the jet noise data of realistic jet engine exhausts. It is also found that these two lobes are generated by two groups of turbulence structures. The peak lobe is generated by turbulence structures traveling at phase speeds greater than ambient sound speed via Mach wave radiation mechanism, which can be observed in Fig. 2 as shown by those arrows. But the downstream lobe is generated by turbulence structures traveling at phase speeds smaller than the ambient sound speed as shown by those closed curves in the same figure. The length scales of the turbulence structures in the first group are in the range of small and medium sizes, but the lengths scales of the second group are very large. It has been speculated that the far-field dual-lobe pattern is generated by an indirect combustion noise source in the public literatures. Our results thus provide an alternative explanation of this dual-lobe phenomenon. Our results also suggest that Mach wave radiation is not exactly a large-turbulence phenomenon as assumed in the past.

Significance: There is a growing need to reduce significantly the noise generated by high performance, supersonic military aircraft. The noise generated during takeoff and landing on aircraft carriers has direct impact on shipboard health and safety issues. The results of our work will provide better understanding of the noise production for both industrial and military aircraft, and will aid the current effort of noise reduction, especially for supersonic aircrafts.

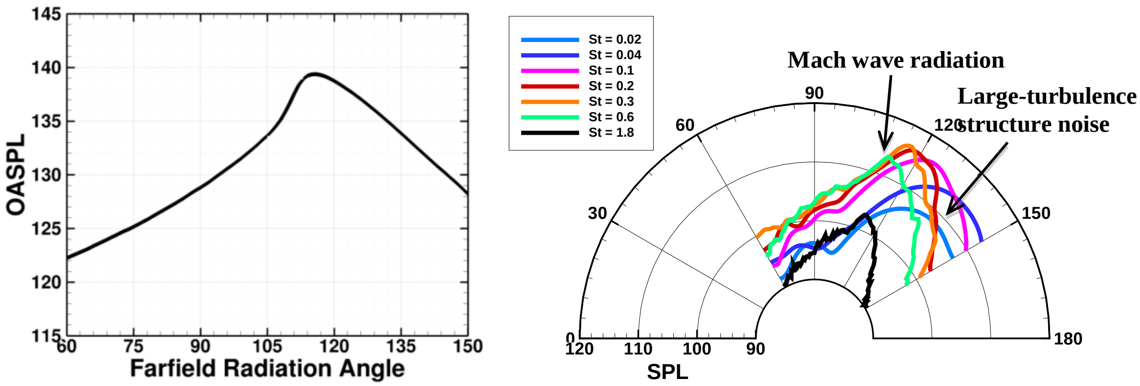


Figure 1. Far-field noise distributions at r = 100D (D is the nozzle exit diameter). St stands for the Strouhal number. (a) Overall sound pressure level (OASPL), (b) Noise level distributions at several frequencies in polar coordinates.

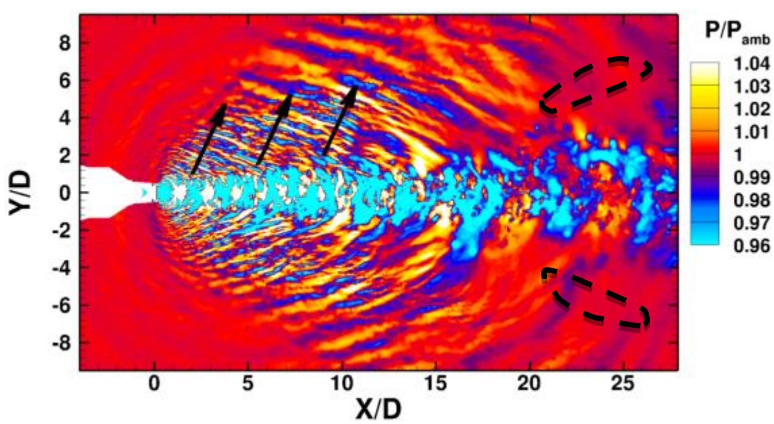


Figure 2. Instantaneous pressure distribution in *XY*-plane at the jet temperature of 2100K. The arrows point to the peak radiation direction of 115° as shown in Fig. 1(a). The closed curves show regions where the very large-turbulence structure noise is visible.

Title: Direct Numerical Simulation of Fluid-Sediment Wave Bottom Boundary Layer
Author(s): A. Levenson, S.P. Bateman, J.A. Simeonov, and J. Calantoni
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CFD

Computer Resources: Cray XE6, Cray XE6m [ERDC, MS]; IBM iDataPlex [NAVY, MS]

Research Objectives: Predictive models for nearshore bathymetric evolution require a complete understanding of the physics of fluid-sediment interactions in the wave bottom boundary layer (WBBL). Since such processes are difficult, if not impossible, to measure in situ, we performed coupled fluid-sediment numerical simulations to increase our understanding of the sediment and hydrodynamics in the WBBL. Fundamental concepts used in describing the phenomena of sediment transport such as mixture viscosity and diffusivity, hindered settling, reference concentration, bed failure criterion, and the concept of acceleration-induced transport are addressed with our models. The models produce high-resolution results necessary to gain insight into the small-scale boundary layer processes and clarify new directions for measurement techniques needed to improve predictive capabilities.

Methodology: Utilization and development of a suite of discrete and continuum WBBL models for simulating sediment transport in the nearshore environment from the microscale (cm-m) to the mesoscale (km) is ongoing with HPC resources. At the microscale (<10 cm), the three-dimensional sediment phase is simulated with discrete element method (DEM) that allows individual grains to be uniquely specified (e.g., size, density, and shape). The fluid phase model varies in complexity from a simple one-dimensional eddy viscosity to a fully three-dimensional direct numerical simulation (DNS). Coupling between the fluid and sediment phases varies from one-way coupling to a system fully coupled at every fluid time step. Also at the microscale (10-50 cm), a continuum model employs a mixture theory approach that simulates the fluid and sediment as a single phase with bulk properties (e.g., viscosity and density) dependent on the local sediment concentration of the mixture. The model solves the unfiltered Navier-Stokes equations for the fluid-sediment mixture and a sediment flux equation that balances gravitational settling, advection, and diffusion. Between the micro- and mesoscale (1-50 m), a spectral seafloor model simulates seafloor roughness dependent on changing wave conditions. At the mesoscale (1-10 km), nearshore hydro- and morphodynamics are simulated with the coupled wave-circulation-morphology model, Delft3D.

Results: We validated the spectral ripple model, NSEA, with time series observations obtained from a 2013 field experiment. The model predicted spectral ripple wavelengths that were in good agreement with observed spectral ripple wavelengths obtained using a fixed platform, high frequency (2.25 MHz) sector scanning sonar. Likewise, the variations in the predicted ripple orientations were similar to the orientations estimated from the sector scanning sonar imagery. Figure 1 shows the model-observation comparisons of seafloor spectra and ripple orientation.

DoD Impact/Significance: Ultimately, all process-based models for nearshore bathymetric evolution are limited by shortcomings in fundamental knowledge of multiphase boundary layer physics. The microscale simulations provide an unprecedented level of detail for the study of fluid-sediment interactions that is impossible to obtain with available measuring technologies in the field or laboratory. These results are utilized to improve parameterizations of small-scale processes in larger-scale models. At the mesoscale, our models are highly efficient and well suited for coupling to regional operational hydrodynamic models in order to include the effects of an evolving seafloor bottom. The computational resources consumed were in direct support of NRL base programs “Modeling Wave Interactions with Arctic Ice Floes,” “Sensing, Observing, and Forecasting High Frequency Resuspension Events in Coastal Proximity (SOFREX),” and “Using remote sensing and numerical models to quantify the role of rip currents in circulation and the resulting sediment transport.”

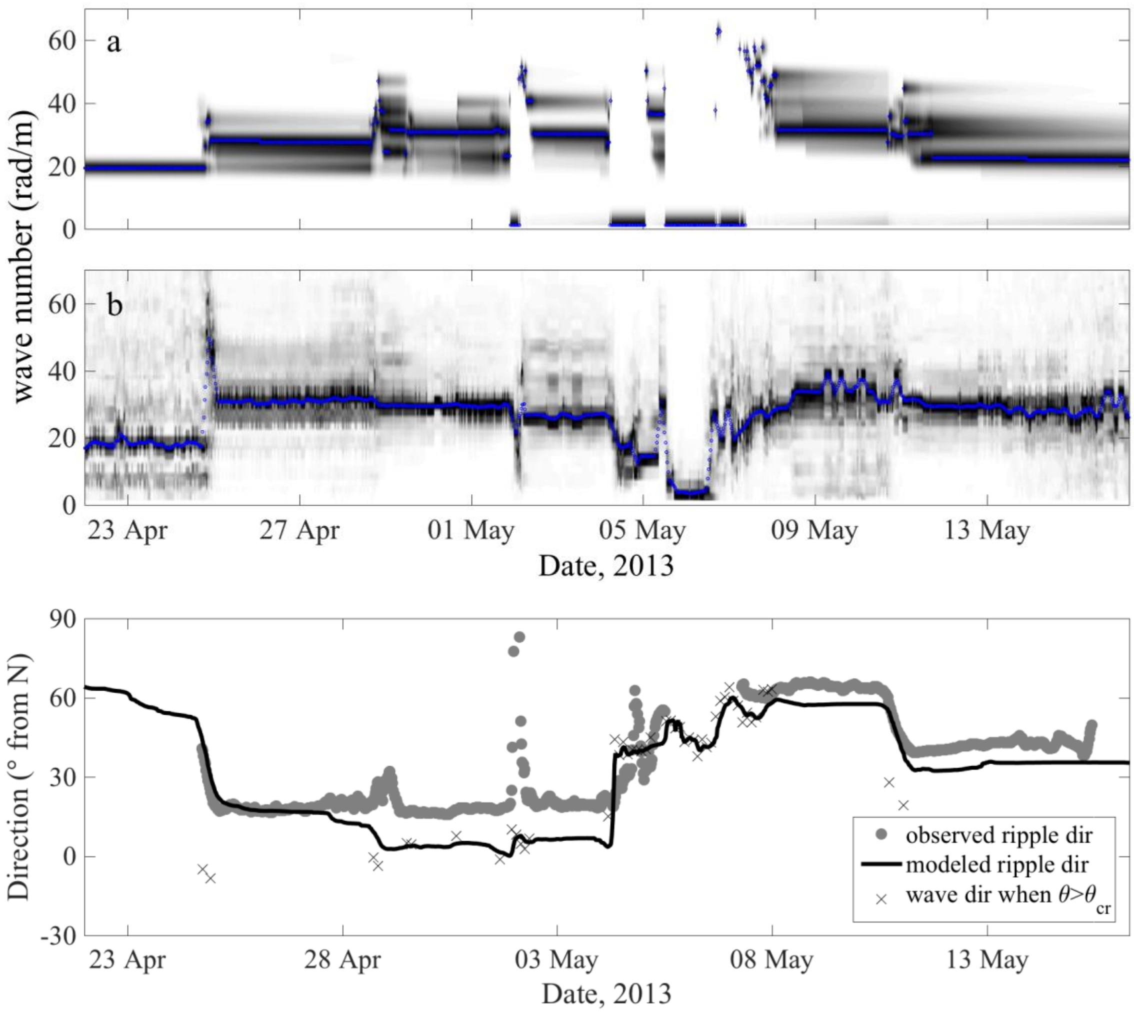


Figure 1. Plots of the one-dimensional seafloor spectra (a) predicted with the model, NSEA, and (b) observed with a fixed platform, high frequency (2.25 MHz) sector scanning sonar. The blue dots indicate the peak wave number. There is very good agreement between the model and observations, especially the times of seafloor change (denoted by an abrupt change in spectra). Energetic wave conditions on 6-7 May 2013 completely washed out the ripples (denoted by very low wave numbers). Plot (c) shows the modeled (solid black line) and observed (gray dots) ripple orientations. The model again agrees well with the observations. Also plotted are the measured wave directions when the waves are energetic enough to affect the bottom. The ripple orientations are closely aligned with the wave direction under the energetic conditions. (Penko et al., *IEEE Journal of Oceanographic Engineering*, 2016)

Title: Particle-in-Cell Simulations of Intense Electron Beam Created Ionization in Air
Author(s): S.B. Swanekamp, A.S. Richardson, I. Rittersdorf, and J.W. Schumer
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: SGI Altix ICE [NRL, DC]

Research Objectives: To develop models for plasma formation and electrical conductivity generation in air during the interaction of an intense electron beam.

Methodology: Recent experiments show that the plasma conductivity depends strongly on the electron-beam current density and the gas pressure. As the pressure and current density vary, the air chemistry kinetics change from a weakly-ionized gas where electrons only interact with the ground unexcited states of the gas to a strongly-ionized gas where the products of the reactions with the ground state are now created in sufficient numbers such that their chemical kinetics are important. Moreover, the plasma electron transport equations are also depend on the gas pressure. At high pressure where the mean-free path between collisions is small compared to density gradient scale lengths, the Boltzmann equation for the plasma-electrons can be approximated by conducting fluid equations with appropriately defined transport coefficients. At low pressures the fluid equations are no longer accurate and the plasma electrons must be treated kinetically. This is accomplished by coupling a Monte-Carlo treatment of electron collisions with the gas to an electromagnetic particle-in-cell code.

Results: Kinetic, time-dependent, electromagnetic, particle-in-cell simulations of the gas transport are being performed to both benchmark the simulations with experiments and to understand the parameter space where simplifying assumptions can be made in both the gas chemistry and the transport algorithm. The simulation geometry is shown in Fig. 1 and is chosen to closely match recent experiments. A typical result is shown in Fig. 2. In these simulations, the plasma electrons and ions collision kinetics are treated from a kinetic Monte-Carlo approach. Plasma motion is modeled using the Lorentz force equation and self-consistent currents are coupled to a Maxwell-equation solver to provide self-consistent electromagnetic fields. The results in Fig. 2 show a significant fraction of the beam current can propagate across the gas-filled cavity. Before this can occur, a significant amount of ionization must occur such that the electron beam's space-charge is neutralized by positive charges in the plasma. This simulation also shows that the ionization fraction is between 1% and 10% (Fig. 2(b)), which indicates that a weakly-ionized gas model is probably not accurate. A more advanced gas-chemistry model is being developed to handle this situation (Ref. 2).

DoD Impact/Significance: The response of air to an intense electron beam pulse has application to the generation and duration of an electromagnetic pulse (EMP). An EMP can result either from a coronal mass ejection directed at the earth or can be manmade from the explosion of weapons and can result in significant damage to sensitive equipment and electronics. The extent of the damage depends on the magnitude and duration of the EMP event which is related to magnitude of the net current defined as the difference between the beam current and the plasma return current.

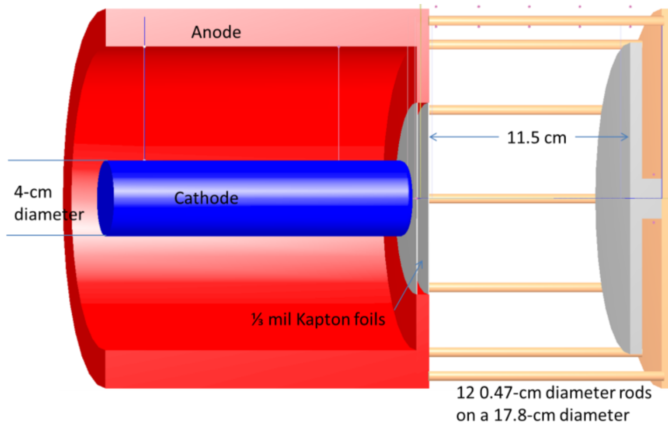


Figure 1. A schematic of electron-beam diode and the gas cell used in the particle-in-cell simulations of the recent experiments.

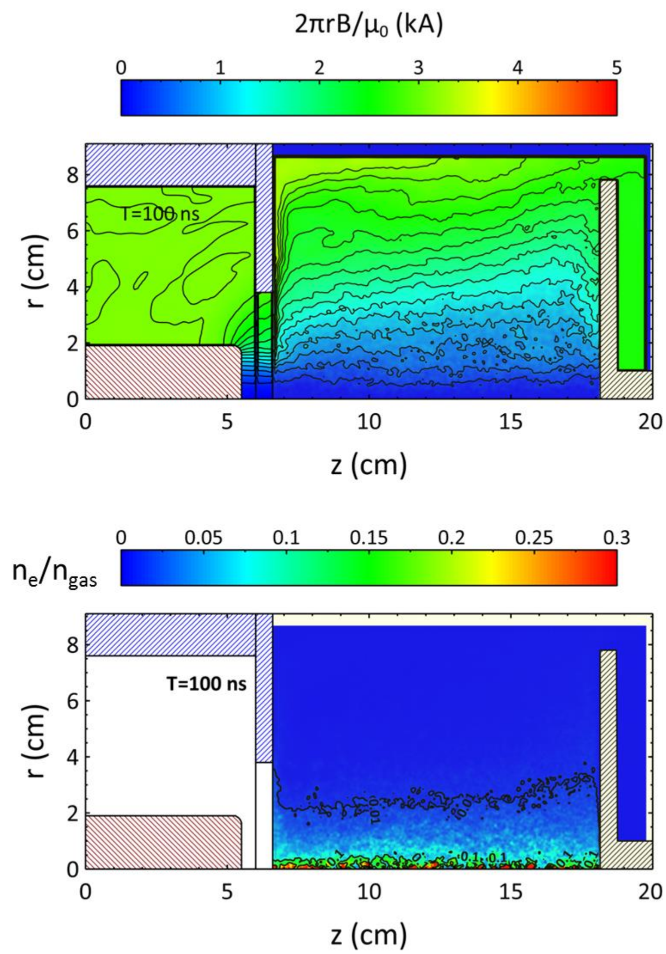


Figure 2. Results from kinetic simulations of gas breakdown for p=100 mTorr and J_b~100 A/cm^2. *Top panel:* Current contours. *Bottom panel:* The ionization fraction.

*This work was supported by the Defense Threat Reduction Agency.

Title: Predicting Fluid-Structure Interaction for Military Applications
Author(s): D.R. Mott
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray XC40 [ARL, MD]

Research Objectives: Create the computational capability to predict the interaction of fluids with flexible structures, including large, high-rate deformations due to blast loading, and convective and evaporative heat transfer at ambient atmospheric conditions. Use the new capability to design novel ventilated body armor components optimized for both blast protection and passive cooling capability. Fully validate the Fluid-Structure Dynamics (FSD) capability by conducting tests on these body armor components and by comparing computational predictions to available validated data.

Methodology: A new discontinuous Galerkin capability for incompressible flows was completed that efficiently computes with high fidelity the low-speed flow about the torso geometries including evaporative cooling due to perspiration. The software package AERO is being used in an interim capacity for materials evaluation and for validation of the evolving software while additional capabilities for computing compressible flow about bodies with large-scale deformation are being developed. The AERO software is open-source and includes an existing capability for modeling fluid-structure interaction that is sufficient to meet many but not all of the modeling requirements of the program.

Results: Research this year focused on completing the incompressible solver within the discontinuous Galerkin framework, and applying this capability to study the flow about idealized elliptical torsos that are partially enclosed in a thin protective armor layer. The primary geometric parameters varied in the study are the amount of armor coverage (i.e., the sizing of openings in the armor that leave part of the ellipse exposed to the ambient wind), wind orientation relative to the body and these openings, and armor stand off (i.e., the distance between the surface of the ellipse and the thin armor layer). The net advection and diffusion of water vapor away from the ellipse was calculated to predict the net cooling provided by each configuration and to assess the impact of varying the primary design parameters that dictate the geometry. For the cases studied, the armor coverage produced the most significant effect on mass transport, but flow orientation can inhibit this effect.

DoD Impact/Significance: Designing complicated, multifunctional equipment for the warfighter such as body armor is a difficult endeavor. Finding designs that simultaneously satisfy competing requirements for providing blast and ballistic protection while providing passive cooling will make our warfighters safer and more effective. The overall computational capability that will arise from this effort will be applied to a range of Navy and Marine Corps applications.

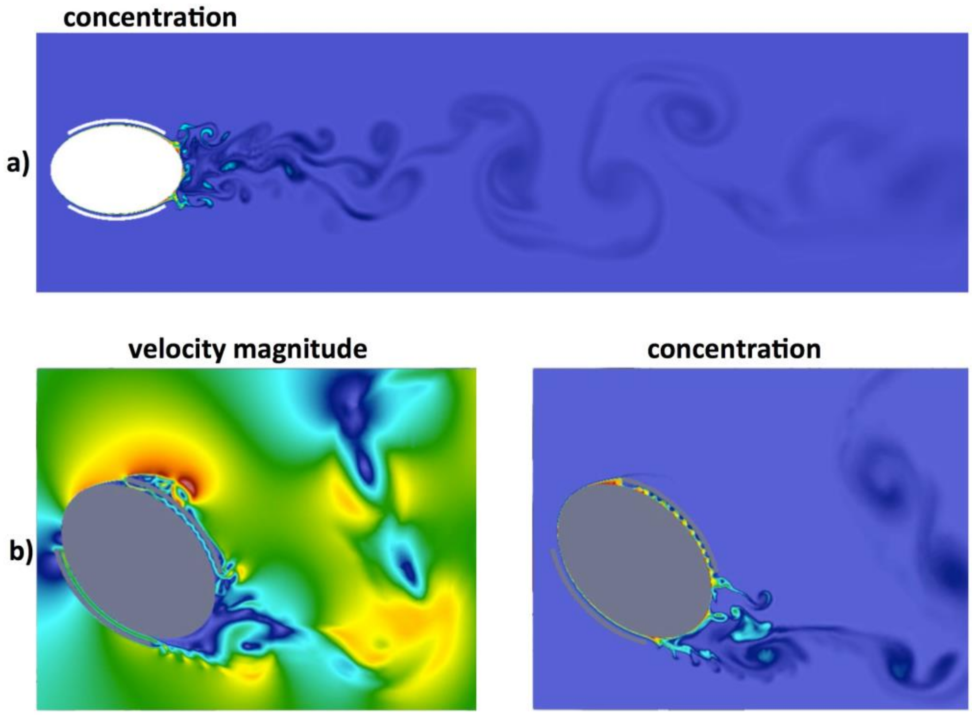


Figure 1. Flow field results from Mott et al. for a baseline torso-armor geometry (3/8 in standoff, 90° exposure as defined in the cited work), at two orientations: (a) concentration distribution for 90° orientation showing the wake, and (b) and velocity magnitude and concentration distributions for 45° orientation showing more detail close to the body. Ambient wind blowing left to right at 5 mph. Velocity magnitude colors range from 15 mph (deepest red) to 0 (darkest blue). Concentration (scaled relative to saturated conditions) ranges from 0 (darkest blue) to 1 (deepest red).

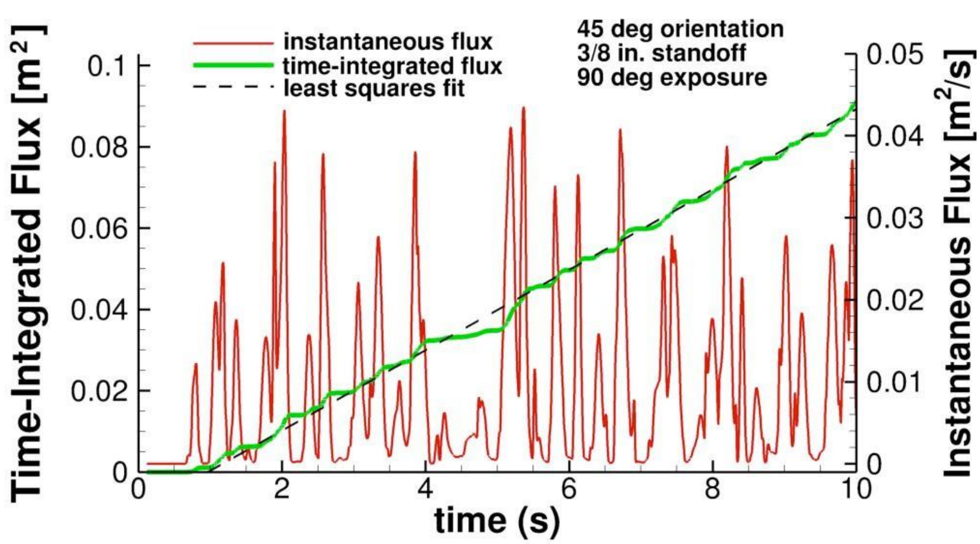


Figure 2. (Mott et al., Fig. 4) Instantaneous and time-integrated flux of the conserved scalar for the baseline case with 45° orientation, 3/8 inch stand off. Shedding from the torso generates a cyclic instantaneous flux, and the slope of the time-integrated flux is used to characterize the average of the instantaneous rate and compare the performance for different designs.

Title: Simulations of the Ionosphere and Magnetosphere
Author(s): J.D. Huba and J. Krall
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CFD

Computer Resources: Cray XE6, Cray XE6m [ERDC, MS]; Cray XC30, SGI ICE X [AFRL, OH]

Research Objectives: Develop space weather forecasting capability. Simulate equatorial spread F, geomagnetic storms, and other events of interest in order to understand the earth's magnetosphere and ionosphere system and to improve the models.

Methodology: The research primarily uses the NRL code SAMI3 which is a comprehensive 3D simulation model of the earth's ionosphere/plasmasphere system covering all latitudes. We have coupled SAMI3 to the inner magnetospheric, ring current code RCM (Rice Convection Model) to study the impact of penetration electric fields on the low- to mid-latitude ionosphere during geomagnetic storms.

Results: A self-consistent modeling study of the ionosphere-plasmasphere system response to the March 17, 2015 geomagnetic storm using the coupled SAMI3-RCM code was performed. We find that the penetration electric fields associated with the magnetic storm lead to a stormtime enhanced density (SED) in the low- to mid-latitude ionosphere. We compare the modeled total electron content (TEC) with GPS measured TEC and find very good agreement. Additionally we observe the development of polar cap `tongues of ionization' and the formation of sub-auroral plasma streams (SAPs) in the post-sunset, pre-midnight sector and its impact on the plasmasphere. However, we did not see the development of plasmaspheric plumes during this event. This research was presented at the 2016 CEDAR/GEM Workshop in Santa Fe, NM. A paper of this subject has been written and will be published in the *Journal of Geophysical Research: Space Physics*.

Measurements show that plasmasphere refilling rates decrease with increasing solar activity while, paradoxically, the vertical integration of the plasmasphere electron density (pTEC) increases with increasing solar activity. Using the NRL SAMI2 (Sami2 is Another a Model of the Ionosphere) and SAMI3 (Sami3 is Also a Model of the Ionosphere) codes, we simulate plasmasphere refilling following a model storm, reproducing this observed phenomenon. In so doing, we find that the refilling rate and resulting pTEC values are sensitive to the oxygen profile in the thermosphere and exosphere: the supply of H^+ in the topside ionosphere is limited by the local O^+ density, through $H + O^+ \rightarrow H^+ + O$ charge exchange. At solar minimum, the O^+ supply simply increases with the O density in the exosphere. At solar maximum, we find that O-O^+ collisions limit the O^+ density in the topside ionosphere such that it decreases with increasing O density. The paradox occurs because the pTEC metric gives more weight to electrons in the topside ionosphere than electrons in the plasmasphere. A paper on this subject has been published in the *Journal of Geophysical Research: Space Physics*.

DoD Impact/Significance: Potential protection of communication satellites and the power grid. Support of ongoing experiments in remote sensing of the space environment. Provide input to ionospheric and thermospheric models.

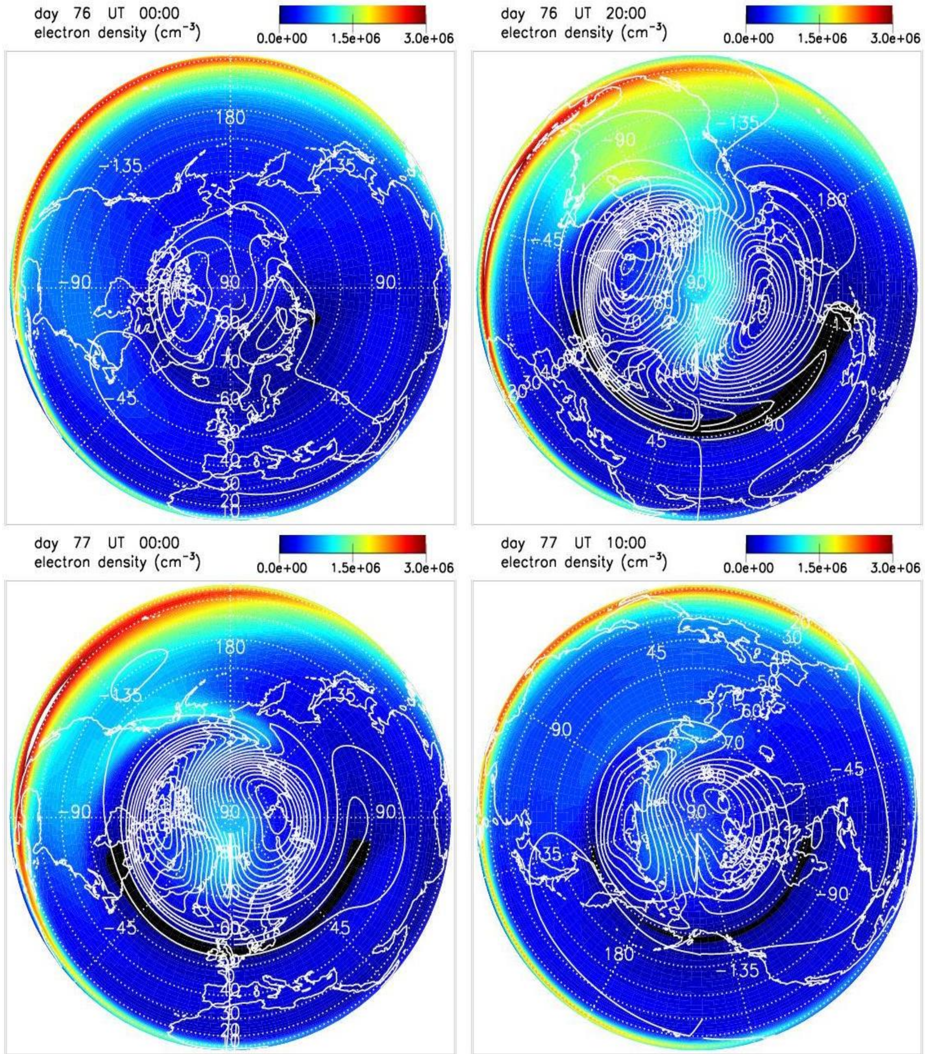


Figure 1. Contour plots of the electron density at an altitude 315 km (colored contours) and electric potential (white lines) before the storm (*top left-hand panel*), during the storm main phase (*top right-hand panel*, *lower left-hand panel*), and recovery phase (*bottom right-hand panel*).

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CCM

Computational Biology, Chemistry, and Materials Science

CCM covers computational tools used to predict basic properties of chemicals and materials, including nano- and biomaterials. Properties such as molecular geometries and energies, spectroscopic parameters, intermolecular forces, reaction potential energy surfaces, and mechanical properties are being addressed. Within the DoD, quantum chemistry, molecular dynamics, statistical mechanics, and multiscale methods are used to design new chemical, polymer, nano- and bio-molecular systems, for fuel, lubrication, laser protection, explosives, rocket propulsion, catalysis, structural applications, fuel cells, and chemical defense. Solid-state modeling techniques are employed in the development of new high-performance materials for electronics, optical computing, advanced sensors, aircraft engines and structures, semiconductor lasers, advanced rocket engines components, and biomedical applications. Of recent emerging interest in the CCM CTA are methodologies that cover bioinformatics tools, computational biology, and related areas, such as cellular modeling.

Title: Non-Collinear Magnetism
Author(s): I. Mazin[1] and J. Glasbrenner[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]National Research Council Post Doctorial Program, Washington, DC
CTA: CCM

Computer Resources: SGI Ice X [AFRL, OH]; Cray XE6 [ERDC, MS]

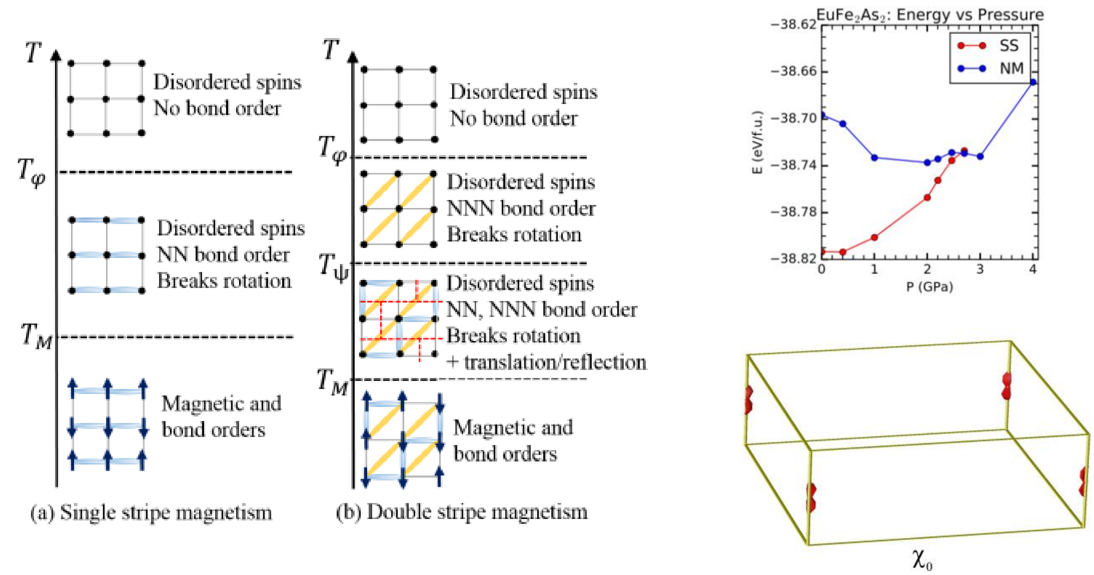
Research Objectives: Understanding physical effects related to noncollinear magnetism, both relativistic and nonrelativistic.

Methodology: We performed first-principles density functional calculations, using the linearized plane wave code ELK and the pseudopotential code VASP at the AFRL and ERDC HPC centers. These codes allow for calculating the total energy for preset magnetic moment directions on each atomic site, as well as full self-consistent relaxation of both the amplitudes and directions of individual magnetic moments, and also calculating total energy of incommensurate magnetic spirals. VASP can be also used to efficiently optimize crystal structures.

Results: (1) We have calculated the total energies of various magnetic supercells and spirals in $BaTi_2Sb_2O$ and mapped them onto a Hamiltonian including (i) Heisenberg terms up to the third neighbors (ii) biquadratic terms up to the second neighbors and (iii) ring exchange. We have shown that this interaction is long-range (third neighbor J and second neighbor K are large), in which case we predict a novel nematic phase diagram that breaks two different symmetries.

(2) In collaboration with the experimentalists, we have investigated energetics and non-interacting spin susceptibility of the high-T_c superconductor $EuFe_2As_2$ under pressure. We concluded that the experimental observation of a rapid shrinking of the tetragonal *c* lattice parameter around 2.7 gigapascals of pressure is due to a discontinuous change in the Fe-As bond length caused by the suppression of magnetism on the Fe sub-lattice. We also confirmed that the wavevector of the magnetic instability still present at 2.7 gigapascals may be on the verge of changing value, correlating with discontinuous changes of the Fe hyperfine field detected by the experimentalists.

DoD Impact/Significance: Bond-order nematicity is one of the most, maybe even the most intriguing discovery in Fe-based superconductors. Perceived earlier as a mathematical curiosity, it was propelled into the spotlight in 2009–2010. Our work raises the stake showing that the nematicity is not limited to one class of materials and to one type of symmetry breaking. Regarding the second project, pressure-induced superconductivity is observed in several pnictide-based superconductors and coincides with the collapse of the lattice *c* parameter. We have shown that the magnetism of one example, $EuFe_2As_2$, changes rapidly in the pressure region close to superconductivity, and that the magnetic order at this point may be of a different kind, which would imply a different type of spin-fluctuation-mediated superconductivity.



Left-hand panel: Schematics of various magnetic and nematic (bond-order) states, possible in Fe-based superconductors (a) or in $BaTi_2Sb_2O$ (b) *Right-hand panel*: Energetics of the stripe antiferromagnetic (SS) and nonmagnetic phases under pressure (top) and the calculated non-interacting spin susceptibility in $EuFe_2As_2$ (bottom).

Title: Calculation of Vibrational and Electronic Excited-State Absorption Spectra of Arsenic-Water Complexes with Water Background Using Density Functional Theory
Author(s): S. Lambrakos,[1] L. Huang,[1] A. Shabaev,[2] and L. Massa[3]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]George Mason University, Fairfax, VA; [3]City University of New York, NY
CTA: CCM

Computer Resources: Cray XC40 [ARL, MD]

Research Objectives: Calculation of vibrational and electronic excited-state absorption spectra of arsenic-water complexes within ambient water background using density functional theory.

Methodology: The present study examines properties of Arsenic-water (As-H_2O) complexes within a water background using quantum theory based calculations and is based on significant progress in density functional theory (DFT), time-dependent density functional theory (TD-DFT), and associated software technology, which is sufficiently mature for the determination of dielectric response structure, and should actually provide complementary information to that obtained from laboratory experiment. This complementary information should be in terms of the physical interpretation of spectral features with respect to molecular structure. The present study adopts the software GAUSSIAN09 (G09) for the calculation of excited state structures.

Results: The results of our study are vibrational and electronic excited-state absorption spectra of Arsenic-water complexes of different sizes, i.e., As-H_2O complexes consisting of 2, 5, 15, 24 and 36 water molecules, within an ambient water background. These studies extend previous studies concerning water clusters of various sizes that considered isolated As-H_2O complexes not within a water background. These results include the relaxed or equilibrium configuration of the As-H_2O complexes' ground-state oscillation frequencies and IR intensities for As-H_2O complex geometries having stable structures, which are calculated by DFT, and excited-state absorption spectra (UV intensities), which are calculated by TD-DFT. A graphical representation of the molecular geometry of an As-H_2O complex consisting of 15 water molecules within a water background is shown in Fig. 1. IR intensity as a function of frequency for this As-H_2O complex is shown in Fig. 2. Oscillator strengths (UV intensity) as a function of excitation energy for the As-H_2O complex consisting of 15 water molecules are shown in Fig. 3.

DoD Impact/Significance: Interpretation of absorption spectra for complexes such as As-H_2O is of significance for detection in practice. This follows in that most environments associated with detection in practice include the presence of water in one form or another, as well as various types of molecular complexes consisting of a contaminant of interest and water. These forms can range from isolated molecular clusters, adsorbed surface layers, droplets and interface regions in liquid phase. Absorption spectra of molecular complexes consisting of water represent a separate regime for dielectric response with respect to electromagnetic wave excitation. This regime should be characterized for improved interpretation of absorption spectra associated with systems that include water complexes as components. It follows that the sensitivity of DFT calculated absorption spectra for molecular complexes, e.g., As-H_2O, with respect to a water background is of significance for qualitative correlation of calculated and measured spectra.

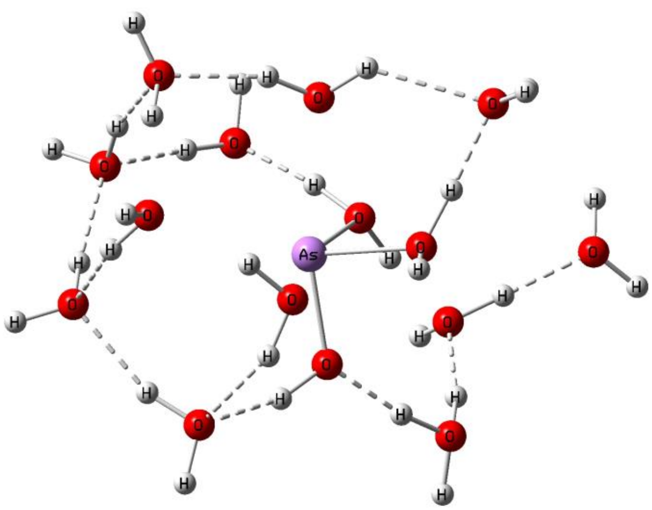


Figure 1. Molecular geometry of As-H_2O complex consisting of 15 water molecules in water background.

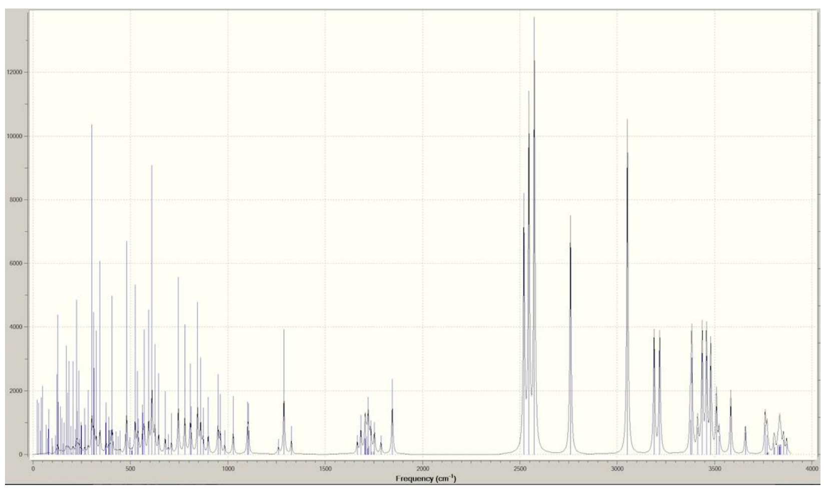


Figure 2. IR intensity as function of frequency for As-H_2O complex consisting of 15 water molecules in water.

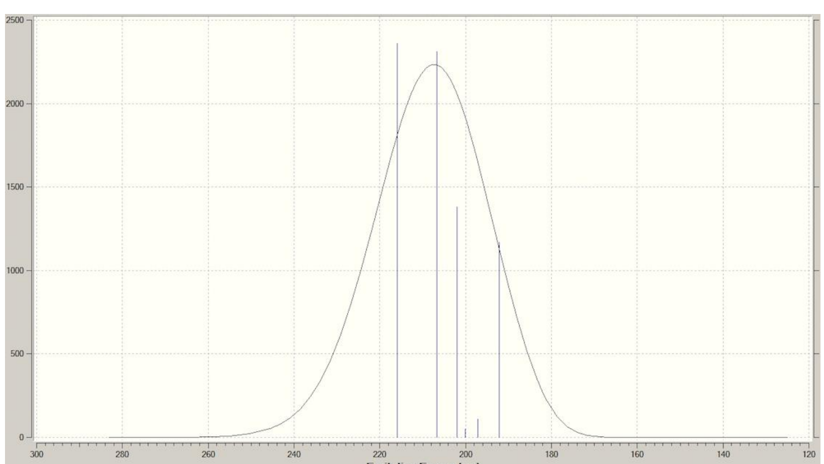


Figure 3. UV intensity as function of frequency for As-H_2O complex consisting of 15 water molecules in water.

Title: First-Principles Simulations of Condensed-Phase Decomposition of Energetic Materials
Author(s): I.V. Schweigert
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: Cray XC40 [ARL, MD]; SGI ICE X, Cray XC30 [AFRL, OH]

Research Objectives: To determine the detailed mechanisms of chemical reactions responsible for decomposition of energetic materials under a wide range of temperatures and pressures.

Methodology: *Ab initio* molecular dynamics (MD) simulations are being used to study chemical reaction dynamics in energetic materials subjected elevated temperatures and pressures. These calculations rely on density functional theory (DFT) to describe changes in the system's potential energy as reactions proceed. Periodic-cell models are used to approximate molecular liquids and crystals under compression. For each model, multiple replicas are prepared using atomic coordinates from experimental or predicted crystal structures and atomic velocities randomly drawn from a canonical ensemble. Each replica is equilibrated using classical (forcefield-based) MD simulations to provide the initial atomic coordinates and velocities for *ab initio* MD simulations. Equilibrated replicas are then rapidly heated using constant-temperature (NVT) *ab initio* MD simulations and the ensuing reactive dynamics is simulated using constant-energy (NVE) simulations. The resulting reactive trajectories are then analyzed to identify which bonds are broken and/or formed as reactions occur. This combination of equilibration, ramp-up, and production runs is expected to provide an adequate sampling of atomic thermal motions, yet eliminate the interference of thermostats with reactive dynamics. A suite of in-house developed scripts that streamline the input deck preparation, job execution, and data analysis is used in these calculations.

Results: This year, *ab initio* MD simulations were completed for initial decomposition reactions in two crystalline polymorphs of RDX—a nitramine energetic compound used in many explosive and propellant formulations. 50 replicas of each polymorph were simulated. For the low-pressure polymorph (α-RDX, Fig. 1(a)), the trajectories were computed for an initial temperature of 1500 K. For the high-pressure polymorph (γ-RDX, Fig. 1(b)), it was found that the rate of decomposition at 1500 K is too slow to be captured within the time scales accessible in *ab initio* MD (picoseconds) and a higher initial temperature of 1750 K was used in the simulations. In both cases, the densities were kept equal to the ambient densities of the polymorphs, respectively, 1.81 and 2.12 g/cm^3. Since no thermostats were used during the production MD simulations, the instantaneous temperature and pressures fluctuated considerably (Fig. 1(c)) as expected for a NVE simulation with a relatively small number of atoms (168). The observed average temperatures and pressures were 1421 K and 2.6 GPa for the α polymorph, 1677 K and 11 GPa for the γ polymorph (Fig. 1(c)). The analysis of the computed trajectories showed that all reactions were unimolecular and homolysis of the weak N-N bonds in RDX (Fig. 1(d)) accounted for most reactions. The simulations also predicted that the radical products of the initial homolysis remained trapped in the "cage" of surrounding molecules and rapidly re-reacted with each other or adjacent unreacted RDX. An example of such a secondary bimolecular reaction is shown in Fig. 1(e).

DoD Impact/Significance: Reaction rate models of condensed-phase decomposition of RDX and other nitramines are needed to support multi-scale simulations of nitramine-based explosives and propellants to impact and shock insults. We have recently derived such a rate model for RDX from the kinetic data available in the literature. One of the key assumptions in the developed model is that the initial reaction mechanism (which is known to be N-N homolysis at ambient pressure) remains the same across a wide range of pressures. The first-principles simulations reported here confirmed that N-N homolysis remain dominant at least up to 11 GPa.

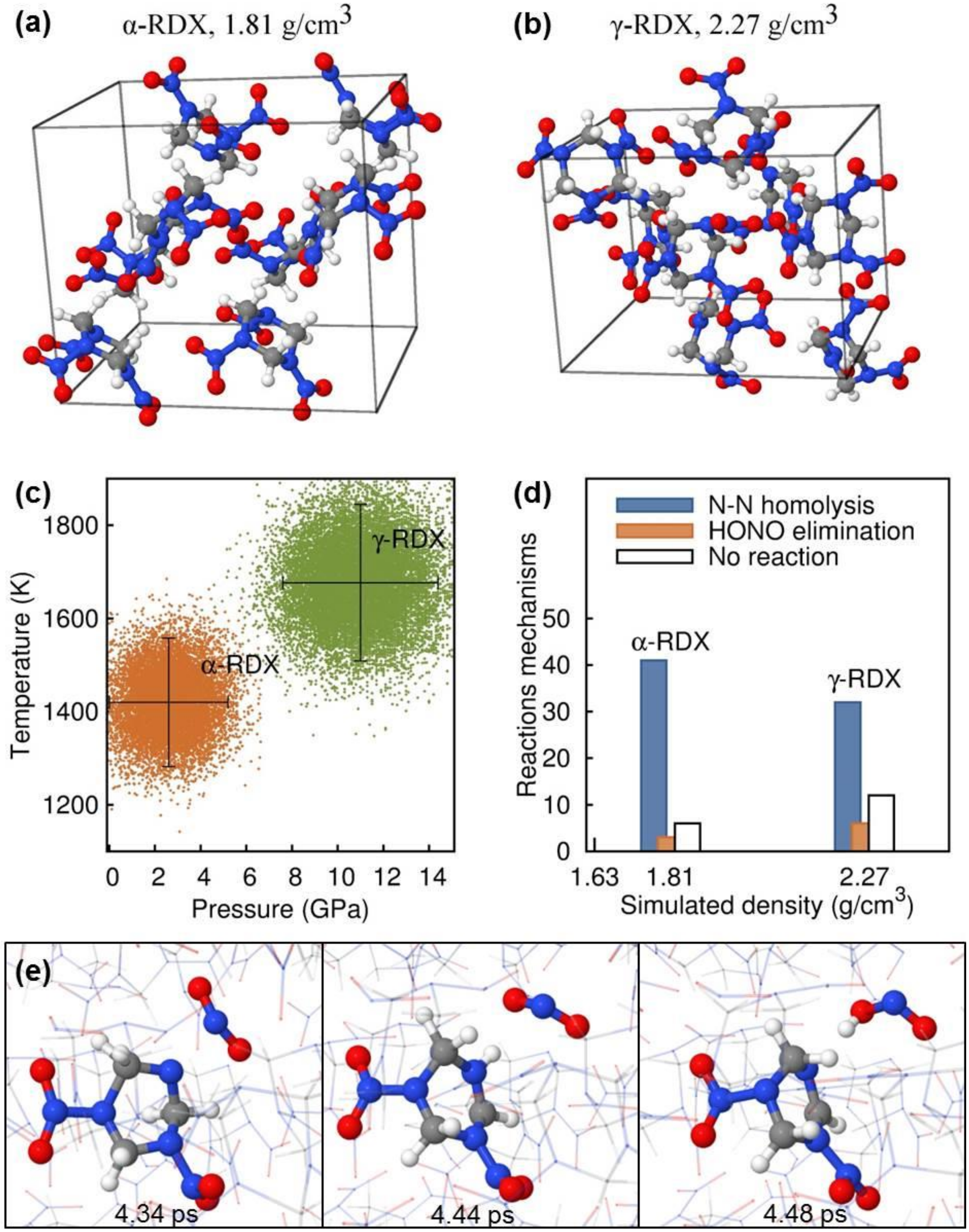


Figure 1. *Ab initio* molecular dynamics simulations of initial decomposition reactions in two crystalline polymorphs of RDX at GPa pressures.

Title: Calculation of Fundamental Physical Parameters for Lower Dimensional Materials
Author(s): C. M. Krowne,[1] N. Cronk,[2] M. Ibrahim,[3] and X. Sha[4]
Affiliation(s): [1] Naval Research Laboratory, Washington, DC; [2] Sotera Defense Solutions, Inc. Herndon, VA; [3] University of Maryland, Baltimore County, Baltimore, MD; [4] Engility Corporation, Chantilly, VA
CTA: CCM

Computer Resources: SGI Altix ICE [NRL, DC]

Research Objectives: The objective is to obtain basic physical parameters of the lower dimensional materials, such as topological insulators (TIs), thin film ferroelectric and ferroic materials, and single or multi-layer graphene, and other lower dimensional materials in 2D or lower.

Methodology: Concurrent with analytical studies using 2nd quantized Hamiltonians, many-body quantum Green's functions, and renormalization techniques, *ab initio* methods are utilized to obtain fundamental parameters including atomic and molecular structure conformation, electronic band structure, charge distribution, and transport characteristics. Various density functional theory codes including ABINIT, Quantum Espresso, CASTEP, and DMOL3 have been used.

Results: Have discovered in a joint ESTD/MSTD program, Lower Dimensional Materials for Naval Applications, metal-insulator transitions in functionalized graphene and RuO_2 nanoskins: M.S. Osofsky, S.C. Hernández-Hangarter, A. Nath, V.D. Wheeler, S.G. Walton, C.M. Krowne, D. K. Gaskill, "Functionalized Graphene As a Model System for the Two-Dimensional Metal-Insulator Transition," *Scientific Reports* **6**, 19939, Feb. 10, 2016; and M.S. Osofsky, C.M. Krowne, K.M. Charipar, K. Bussmann, C.N. Chervin, I.R. Pala, and D.R. Rolison, "Disordered RuO2 Exhibits Two Dimensional, Low-Mobility Transport and a Metal-Insulator Transition," *Scientific Reports* **6**, 21836, Feb. 26, 2016. Materials growth, measurements and quantum diagrammatic quantum field studies had been conducted for graphene to study its metal-insulator transition (MIT). DFT calculations have been performed to examine the surface features of the TI material Bi_2Se_3 (see Fig. 1), focusing on the scanning tunneling microscopy imaging using two different CCM codes: CASTEP and Quantum Espresso combined with XCRYSDEN, aiming to understand the origin of the coexistence of impurity- induced quasi-one-dimensional electronic structure and topological surface states in doped Bi_2Se_3, as shown in recent experiment. See Fig. 2 for examples of 2D material quantum transport properties, measured in terms of quantum resistance units h/e^2, the type of systems we are examining.

DoD Impact/Significance: Lower dimensional materials hold promise for moving technology into the realm where conventional devices and materials cannot perform, which is of great importance to the Navy and DoD. For example, since graphene material does display an MIT, then many new solid state microscopic devices could be envisioned which require switching capabilities, avoiding or supplementing those being pursued with phase change materials, such as vanadium dioxide, which require inconvenient temperature changes. Likewise, transparent conductive materials like RuO_2 nanoskins, which display an MIT, could be used in many device contexts, from solar cells to transistors. MIT materials could even be used as shields against incoming interrogating radiation, because they transition under dc electric E fields or even under rf fields, not only under temperature changes. For TIs, this may provide another way to develop 2D type of transport materials with a substrate, removing the problem with how to handle single layer atomic materials like graphene.

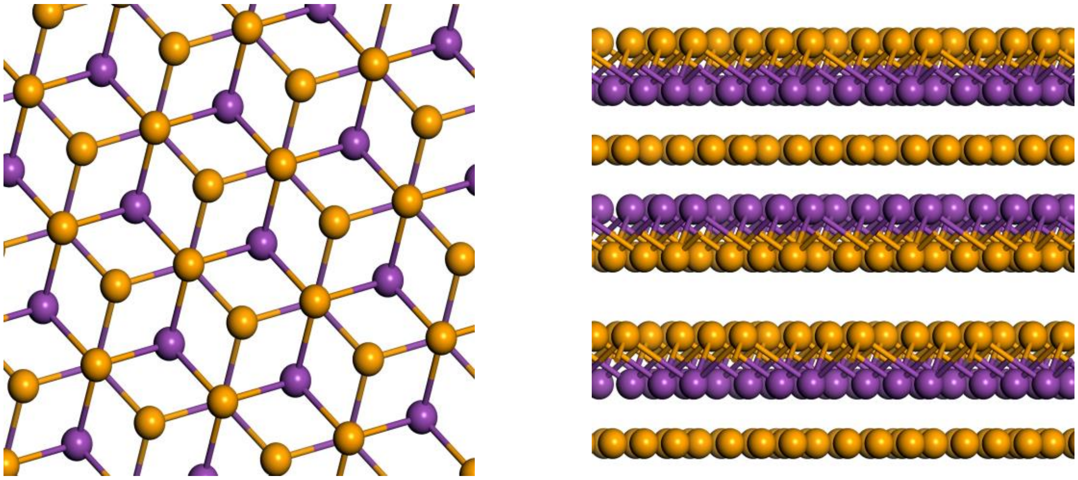


Figure 1. Top and side views of the (0001) surface of the topological insulator Bi_2Se_3 (where gold denotes Se atoms, and purple Bi atoms).

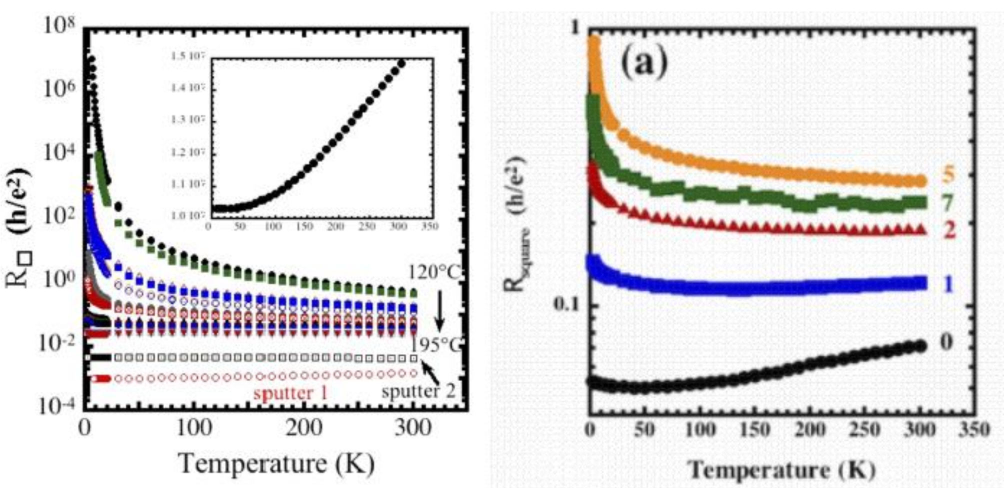


Figure 2. *Left-hand graphic:* Sheet resistance versus temperature of thin film disordered and crystalline RuO_2, plotted in terms of quantum resistance h/e^2. *Right-hand graphic*: Resistance per square for graphene exposed to nitrogen, same units.

Title: Growth and Control of Metal Films on Semiconductor Substrates
Author(s): S.C. Erwin
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI ICE X [AFRL, OH]

Research Objectives: To explain theoretically the atomistic surface morphology and the electronic and magnetic structure of Si(775)-Au, a reconstructed surface of silicon in the broader family of surfaces Si(*hhk*)-Au. Some members of the family form “silicon spin chains” at the step edges of these terraced surfaces, while Si(775)-Au does not. Understanding these differences could lead to the ability to create and control silicon spin chains.

Methodology: We used density-functional theory (DFT) with the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE), and with the generalized-gradient approximation of Perdew, Burke, and Ernzerhof (PBE). The best approach for the problems studied here is the projector-augmented-wave (PAW) method as implemented in the VASP code.

Results: We demonstrated theoretically as well as experimentally that the Si(775)-Au surface has—despite its very similar overall structure to spin chain systems such as Si(553)-Au and Si(557)-Au—zero spin polarization at its step edge. Using a combination of density-functional theory and scanning tunneling microscopy, we proposed an electron-counting model that accounts for these differences. The model also predicts that unintentional defects and intentional dopants can create local spin moments at Si(*hhk*)-Au step edges. We analyzed in detail one of these predictions and verified it experimentally.

DoD Impact/Significance: This finding opens the door to using techniques of surface chemistry and atom manipulation to create and control silicon spin chains. Our model of spin creation and destruction by hole and electron doping, respectively, motivates us to propose using surface chemistry to create and manipulate spin chains. For example, one can envision using atom manipulation techniques to create and arrange adatom vacancies on Si(775)-Au, and hence to construct spin chains with tunable lengths and spacings. In addition to the native defects investigated here, a large class of foreign adsorbates offers broad opportunities—depending on their electronic character—for inducing or suppressing step-edge spins at Si(*hhk*)-Au surfaces. Finally, it is likely that our results and proposal for controlling spins at the steps of Si(*hhk*)-Au are also relevant—probably with interesting modifications—to many other related materials systems, such as silicene or germanene, as well as to other physical configurations, such as finite ribbons.

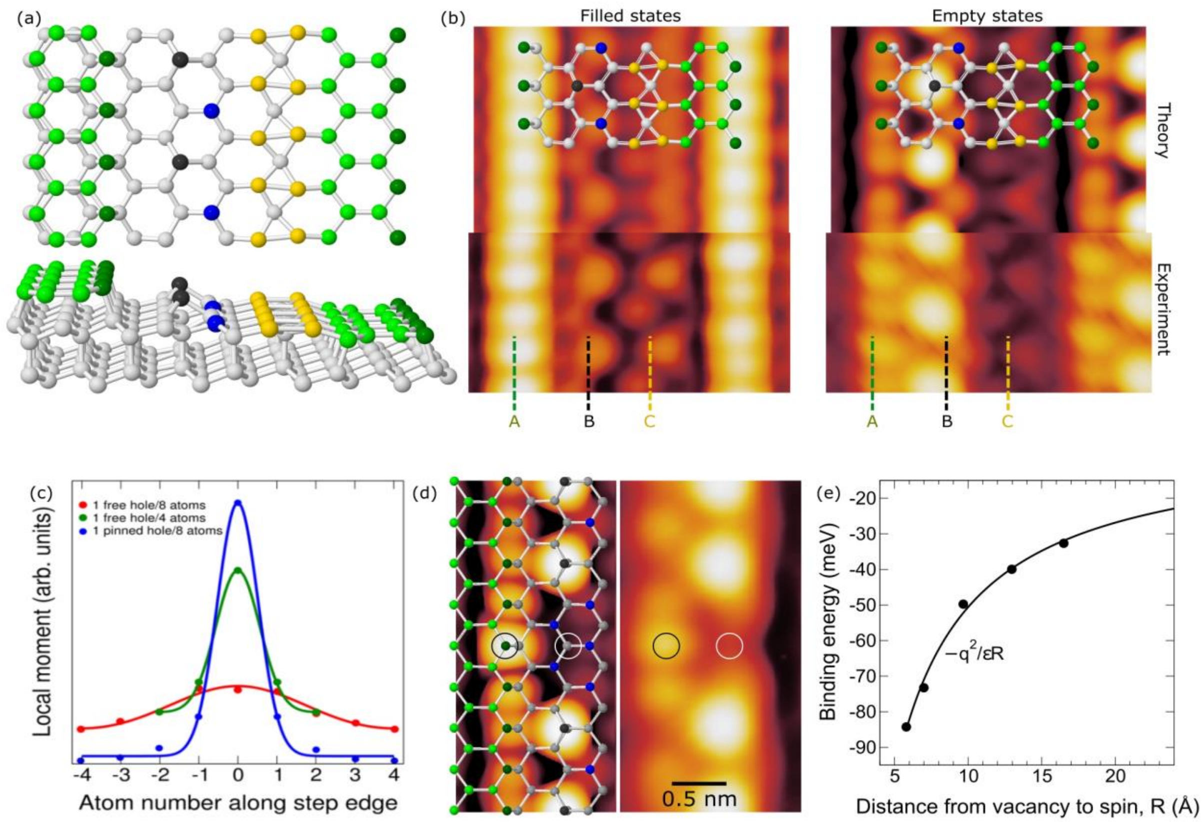


Figure 1. (a) Proposed structure of Si(775)-Au. Yellow atoms are Au; all others are Si. Each terrace contains a Au double row and a graphitic Si honeycomb chain (green) at the step edge. The ladder structure of the Au row has doubled periodicity due to an alternating twist of the ladder rungs. A row of Si adatoms (black) with doubled periodicity passivates three surface dangling bonds per 1x2 cell, leaving one unpassivated Si restatom (blue) per 1x2 cell. All of these effects give rise to discernible features in the STM topography. (b) Comparison of experimental (lower) and simulated (upper) STM images for filled and empty states (experimental bias −1.0 and +1.0 eV, theoretical bias −0.8 and +0.8 eV).
(c) Theoretically predicted formation of spin moments when holes are added to Si(775)-Au. When added at low concentrations, the resulting spins partially delocalize along the step edge; compare the cases of one free hole per 8 step-edge atoms (red) and per 4 step-edge atoms (green). Holes can also be pinned by their electrostatic attraction to a nearby charged defect (here, the adatom vacancy in panel d). In this case the spin is more strongly localized (blue). Curves are Gaussian fits to DFT local magnetic moments. (d) Simulated and experimental empty-state STM images of an adatom vacancy (white circle) on Si(775)-Au. The vacancy adds one hole, which renders the nearest step-edge atom (black circle) spin-polarized and hence brighter in STM. (e) Theoretical electrostatic binding energy of the negatively charged adatom vacancy to the positively charged step-edge spin. The lowest energy configuration, with binding energy 85 meV, is realized in d.

Title: Surfaces and Interfaces in Oxides and Semiconductors
Author(s): C.S. Hellberg
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

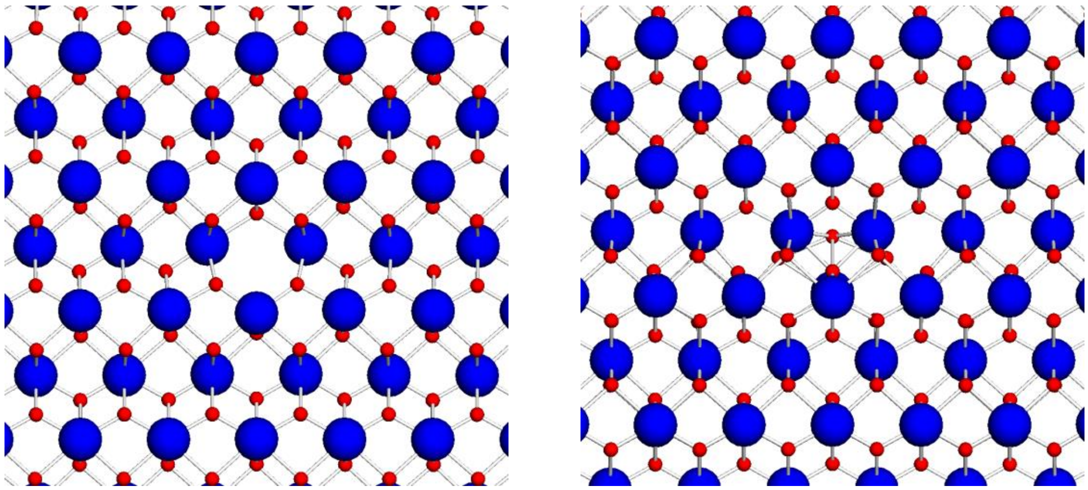
Computer Resources: SGI ICE X, Cray XC30 [AFRL, OH]; Cray XE6 [ERDC, MS]; Cray XC40 [ARL, MD]; SGI Altix ICE [NRL, DC]

Research Objectives: Determine the source of the lattice expansion observed during flash sintering. Application of a weak (< 200 V/cm) external electric field has been shown to increase the rate and reduce the temperature of sintering in many ceramics, a phenomenon named flash sintering. Recent work has performed continuous x-ray diffraction on Yttria Stabilized Zirconia (YSZ) during the sintering under an applied field, finding a sudden and approximately uniform increase in the lattice constants of the sample (but no phase transition) accompanied by a sharp increase in the conductivity. When the conductivity reaches a critical value, the applied field is turned off, and the lattice constants recover at approximately the same rate that they increased. The width of the (112) diffraction peak reduces at the point of expansion, and remains smaller after contraction, while the width of the (211) peak remains nearly constant. Similar behavior has been observed in other ceramics including B_4C and $BaTiO_3$.

Methodology: We performed first-principles density functional calculations to determine the lowest energy Frenkel defects (vacancy-interstitial pairs) in Zirconia. We used the VASP planewave code at the AFRL and ERDC HPC centers. This code allows a system with many atoms (we used up to 384 atoms) to be simulated and, most importantly, relaxed accurately.

Results: We find that the Frenkel defect causes the lattice constant in our calculations to expand. Additionally the *a* lattice constant of the tetragonal unit cell increases more than the *c* lattice constant, in agreement with the *in situ* x-ray diffraction results.

DoD Impact/Significance: Flash sintering occurs much faster and at significantly lower temperatures than conventional sintering in most, but not all ceramics. Flash sintering was only discovered in 2010, and is expected to improve the processing of these materials. By understanding the microscopic mechanisms that contribute to flash sintering, we may be able to improve the process even further and also to modify the technique so that it can be used on materials that do not currently respond to the applied electric field, such as Al_2O_3.



The two defects that comprise an oxygen Frenkel pair in ZrO_2. Zr atoms are blue, and O are red. (a) The oxygen vacancy. (b) The oxygen interstitial. Only atoms within slab of width 0.8 nm are shown for clarity.

Title: Biomolecular Conductance: Principal Component Analysis of *G. sulfurreducens* Cytochrome-c
Author(s): N. Lebedev
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI ICE X [AFRL, OH]

Research Objectives: Bacterial electroactive biofilms (BF) attract researchers' attention due to their ability for generation of electric current when electrons travel for very long distances, up to several tens of microns in the course of cell metabolic activity. It was demonstrated that this electron transfer (ET) correlates with the accumulation in the BF of huge amounts of a c-type cytochrome (Cyt), but molecular nature of this Cyt, its spatial localization, interaction with the environment, regulation and the controlling factors are not completely understood. This problem can be solved by computer simulation of Raman spectra allowing for identification of their structural origin and project/map them to molecular structure at sub molecular spatial resolution. Principal Component Analysis (PCA) allows for data squeezing to smaller number of the main, so called principle, components (PCs). Prescribing these PCs to specific classes of molecules allows for classification and comparative analysis of complex systems.

Methodology: Biological macromolecules, particularly proteins, consist of thousands of atoms and their calculation can be achieved only with the power of HPC. To solve the problem, in our PETTT project we substantially modify the software for the calculation of molecular conductance by massive parallelization. In our calculations, electronic structure optimizations are performed with Gaussian09 using a density functional theory (DFT) approach with a nonlocal exchange correlation functional comprised of Becke's three-parameter exchange functional and the Lee−Yang−Parr correlation functional (B3LYP) with a Lan2DZ polarized basis set for iron and 6-31G(d) basis set for the rest of the heme. This calculation allows us for prescribing (projecting) individual vibrational modes detected in experimental Raman spectra to specific parts of the protein. For identification of the role of these modes in Cyt functional operation we perform Principal Component Analysis of the Cyt Raman spectra obtained at various experimental conditions. By rotating of the principle component axis (Exploratory Factor Analysis) we are able to achieve better orthogonality of individual components and their projection to heme structure with sub molecular spatial resolution. The initial design and estimation of the heme molecular structure, molecular orbital (MO) energies and spatial distributions is performed on personal computers, while scaling up these results to large systems is performed using HPC (Spirit).

Results: Computer simulation of Cyt Raman spectra reveals about 20 main Raman modes that are due to heme collective oscillations. PCA shows that these vibrations can be squeezed to three principal components (describing about 86% of the protein response to the environmental factors) one of which is sensitive to the protein location within the bacterial cell, and the other indicates the cell interaction with the environment, particularly binding to inorganic substrate.

DoD Impact/Significance: The obtained results give a quick and reliable tool for identification of bacterial cell-substrate binding and ET activity from experimental Raman spectra.

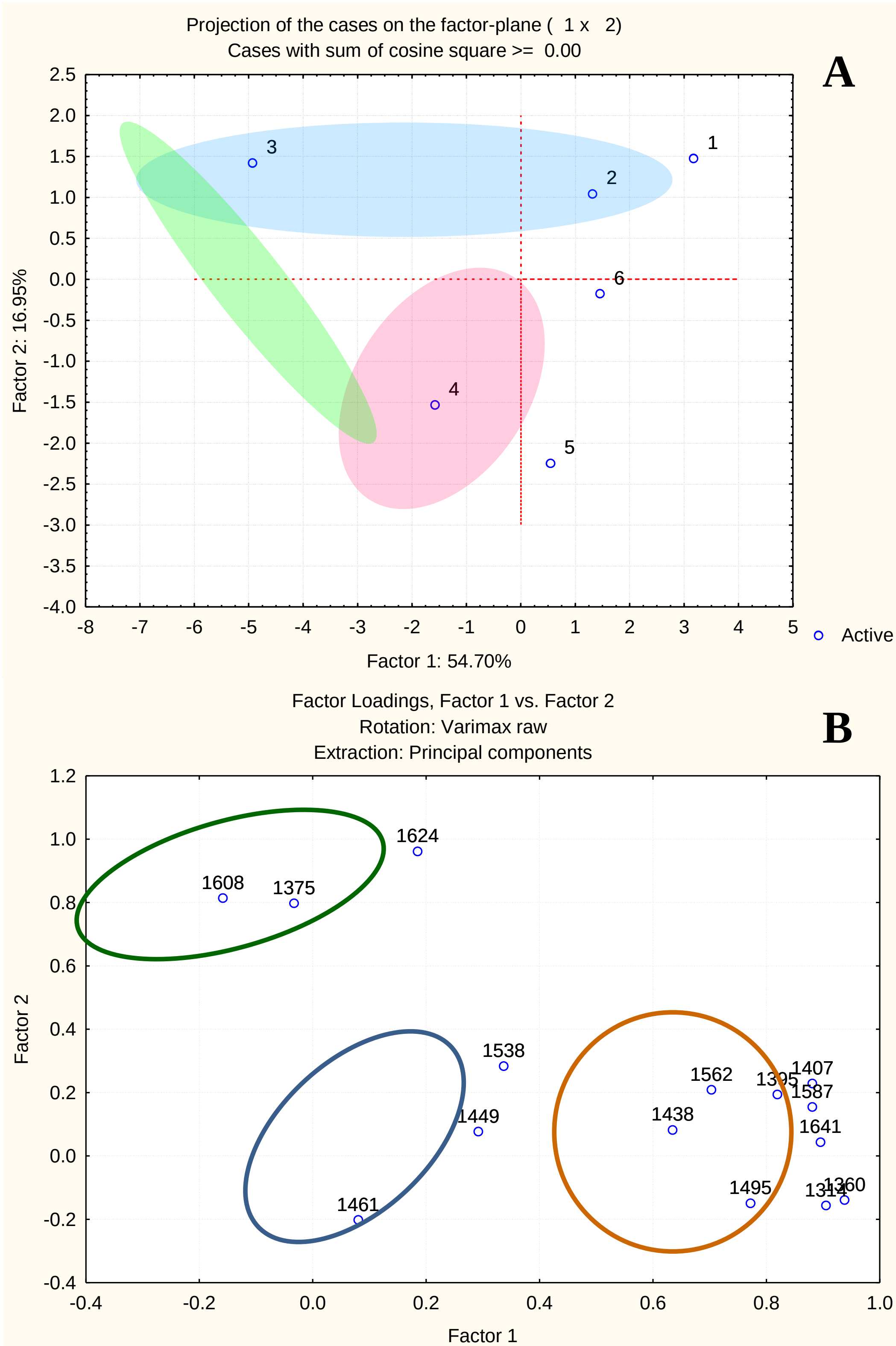


Figure. (A) Identification of intracellular and surface exposed Cyt (+ and – signs of factor 1) and bacterial cell interaction with the substrate (+ and – signs of factor 2) in *G. sulfurreducens* biofilm on a mineral (mica). (B) Classification of the Cyt Raman bands (numbered by the position of their maxima) into three principal components (circled with brown, blue, and green).

Title: Materials for Energy Storage and Generation
Author(s): M. Johannes
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI ICE X, Cray XC30 [AFRL, OH]

Research Objectives: The objectives of this program are to use density functional theory (DFT) to understand the properties and performance of energy storage and generation materials, especially with respect to nanoscale effects, defects and interfaces.

Methodology: First principles pseudopotential methods are employed to calculate the quantities of interest. The majority of the work was done using the Vienna Ab initio Software Program (VASP), but a substantial minority was done using the Wien Code which is a full-potential LAPW code. Post-processing is done using personal codes. Both standard (static)T=0 DFT calculations and temperature-dependent molecular dynamics (MD) calculations were used.

Results: In FY16, the majority of work on this project involved modeling the ionic and electronic conduction properties of nanoscale alumina coatings. Since alumina is in the bulk and under normal conditions both an insulator and an extremely bad ionic conductor, it is still a mystery how electrons and ions can pass through a coating during electrochemical cycling, as has been experimentally shown. Our results show that saturating the coating with Li ions (not atoms!) causes a space-charge build-up, which significantly lowers the energy barrier for Li ion hopping within the coating. This explains the mechanism itself as well as the necessity for the nanoscale nature of the coatings: reasonable diminishment of Li supplies at saturation.

There has also been significant continuing work on the role of defects in the electrochemical behavior of transition metal oxide materials used as Li ion battery cathodes. Our work this year uncovered the role of intentional Al defects (very low level doping) in 3d-based cathode materials. It has long been recognized that such doping improves the stability of such materials at very low doping but after a critical level, drastically reduces the capacity and performance. By calculating the structure, electronic structure and defect energies of Al-doped materials, we showed that at low concentrations, the Al does indeed stabilize the material via charge transfer away from unstable 3d metal ions. However, at concentrations high enough that Al can be situated in the Li plane between two 3d plane defects, it pulls the transition metal planes together, lowers the defect energy and starts a runaway process of increased dopant intercalation and contraction that severely reduces ionic mobility.

Finally, work on superconductivity continued with an emphasis on the role of spin-orbit effects in nominally two-dimensional materials. By comparing two Pd-based superconductors we found that spin-orbit coupling at the Pd site largely controls the dimensionality by locking the spins to the lattice. Since the Pd content is variable (within some constraints), this means that the superconducting dimensionality can be manipulated via Pd variation.

DoD Impact/Significance: Alumina coatings on electrode materials, particularly when both the underlying material and the coating are in the nanoscale regime, is a very promising avenue for stabilizing electrodes against degradation under electrochemical conditions. Understanding the precise parameters that control the crucial properties of electronic and ionic conductions renders these coatings practically useful. And in fact, using knowledge derived from these calculations, an actual coated graphite electrode that could withstand 200% overcharging was synthesized and tested. The resistance to overcharge is relevant to safety, as accidental overcharge is what causes dendrite formation, chemical instability, and eventually short-circuit or catastrophic failure (fire).

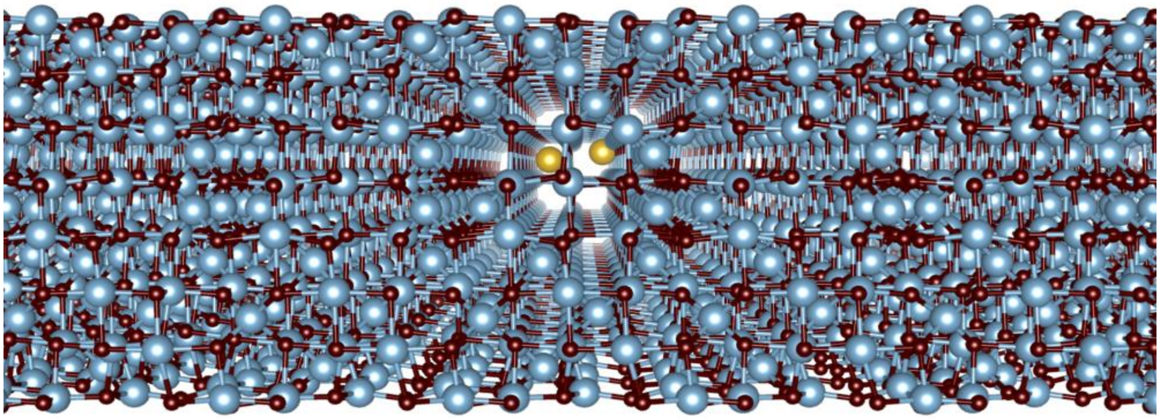


Figure 1. Li ions diffusing through a nanoscale alumina coating

Title: Multiple Length and Time Scale Simulations of Material Properties
Author(s): N. Bernstein
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

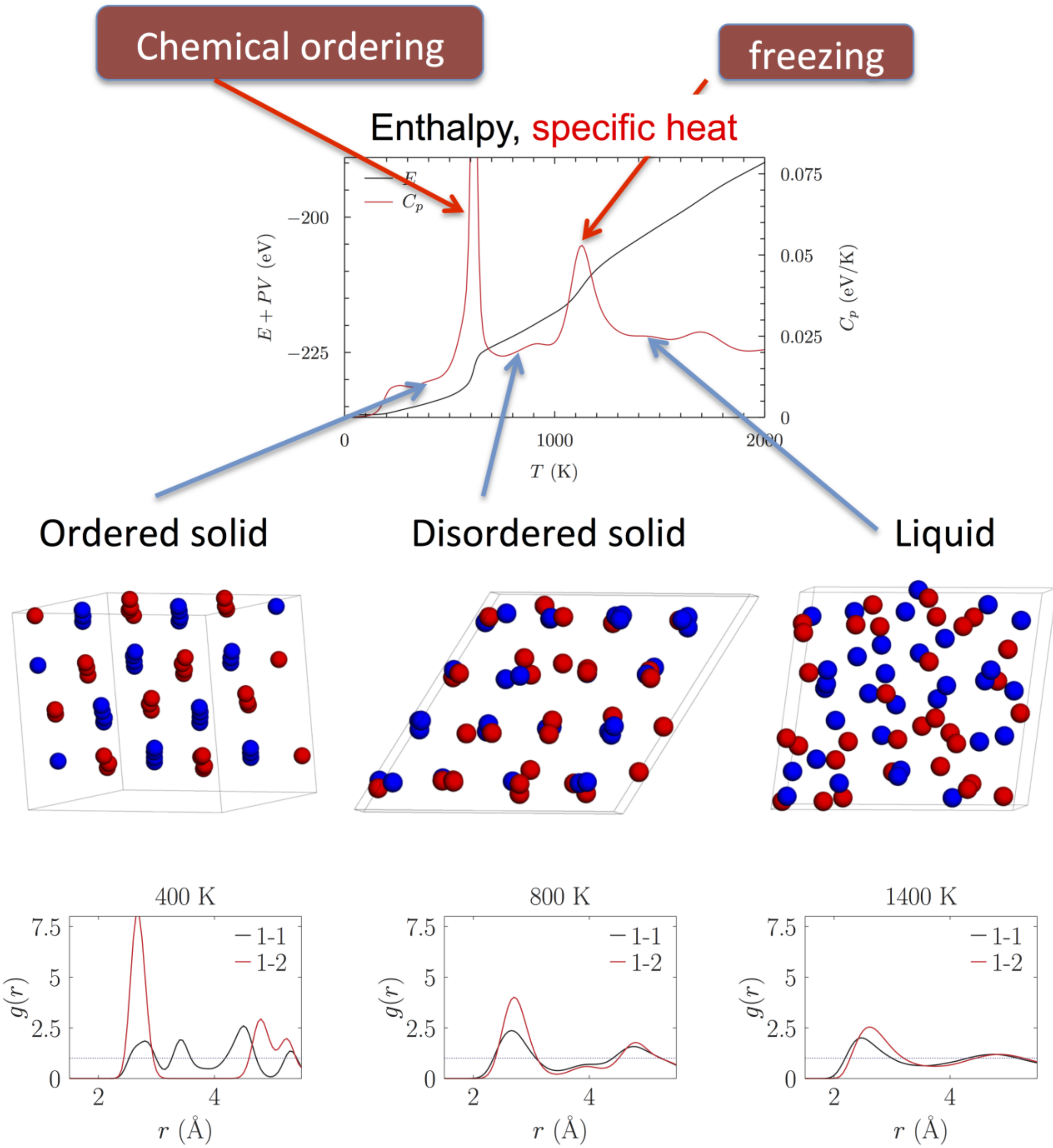
Computer Resources: Cray XC40 [ARL, OH]; SGI ICE X [AFRL, OH]; [ERDC, MS]

Research Objectives: To understand and predict mechanical, structural, and energetic material properties.

Methodology: Molecular dynamics (MD) and Monte Carlo (MC) for the time evolution and sampling of atomic configurations. Trajectories use energies and forces from density functional theory (DFT) and interatomic potentials. Nested sampling used for calculating thermodynamic quantities and phase diagrams. Numerical integration of $k \bullet p$ electronic structure model for Auger recombination rates. The software implementing these methods included VASP for DFT simulations, LAMMPS for interatomic potential MD, ASE and libAtoms/QUIP for interfacing between various programs, and pymatnest for nested sampling. Matlab was used for numerical solution of Auger recombination rates in nanostructures.

Results: The development of a potential for silicon with the Gaussian Approximation Potential (GAP) machine-learning-based method was continued. As a test, the Si GAP was used for thermal conductivity calculations with the Green-Kubo method implemented in the LAMMPS code. These show promising agreement with DFT calculations (using the Boltzmann transport equation approach) at moderate temperatures. Work on a different computational method, nested sampling for configuration space exploration and thermodynamic quantity calculations, consumed the majority of the computational time. This new method shows great promise for calculating phase diagrams for condensed phases with a minimum of parameter tuning, only a few systematically convergeable parameters that appear to be fairly transferable between different materials. A large set of runs testing convergence rates and performance on a range of model systems, including monoatomic and binary Lennard-Jones potentials, an embeded atom CuAu potential, and the modified embedded atom Ti potential were completed. In addition to this method development, two other systems were simulated. The first is Ti, where the VASP DFT code was used to carry out vibrational density of states (vDOS) calculation at finite temperature. From the vDOS the stability of different phases (hcp, α, and bcc, β) as a function of temperature will be extracted. The second system is a cylindrical nanostructure where non-radiative decay of excitons was calculated from a simple model of the electronic structure. Matlab Distributed Compute Engine was used to carry out the large scale numerical solution of the derived differential equations.

DoD Impact/Significance: Machine-learning based interatomic potentials such as GAP approximate the DFT energy with much lower computational cost. These could revolutionize atomistic simulations of many systems which are currently too chemically complex to simulate with interatomic potentials, but too structurally complex for the system sizes that are tractable with DFT. The nested sampling method provides robust method for thermodynamic properties and phase diagrams, without the critical slowdowns at phase transitions that affect currently used methods. This prediction capability is essential for determining the stable phases that control the properties of new and improved materials. Ti is lightweight and corrosion resistant, of great use as a structural material for naval applications. Controlling its plasticity, which is greatly affected by its atomic structure, is important for developing processes such as friction-stir welding needed for its use in applications. Nanoscale semiconducting systems can be used as photon sensors and light emitters, but non-radiative Auger recombination processes reduce their efficiency. Simulating these processes for realistic geometries, including the materials' electronic structure, is essential for improving their performance in light-related applications.



Results of a nested sampling run for binary LJ with tendency for chemical ordering. *Top panel:* Enthalpy and specific heat as a function of temperature, with two specific heat peaks corresponding to transitions indicated in the figure. *Middle panel*: Representative configurations from each temperature range, from left to right: above freezing (liquid), below freezing (chemically disordered solid), below chemical ordering (chemically ordered solid). *Bottom panel*: Radial distribution functions with same (1-1) and different (1-2) chemical species ordering from ensemble averages at the same three temperatures.

Title: Marine Biofilm Metaproteomics
Author(s): W.J. Hervey IV, A. Jackson, and G.J. Vora
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: Cray XE6, Cray XE6m [ERDC, MS]; SGI UV [AFRL, OH]; SGI Altix ICE [NRL, DC]

Research Objectives: To implement a modular data analysis pipeline of selected open-source software applications for biomolecular characterization of marine biofilm and biofouling microbial consortia. Integration of disparate, large-scale data tiers of biological information on genomic, transcriptomic, proteomic, and metabolomic levels is a prerequisite to understanding biofilms at the molecular level. At present, a large number of organisms are not cultivatable under laboratory conditions due to lack of understanding of their fundamental metabolic processes. Formidable computational challenges in this multidisciplinary research area include an unprecedented rate of data acquisition and rapidly evolving commercial analytical platforms. Thus, it is necessary that data analysis methods be both computationally robust and modular in nature (i.e., constructed of separate software programs that may be continuously evaluated and interchanged as necessary) such that it may be modified accordingly with technological developments in each "-omics" sub-field, adapted to new experimental goals, and scaled to emerging HPC architectures.

Methodology: The process of creating large-scale metaproteome inventories of proteins predicted to be present among marine biofilms is three-fold: assembly of small DNA pieces into larger contiguous segments, prediction of protein-coding regions from contigous DNA segments, and *in silico* translation of the genetic information into protein sequence data. Two factors make this workflow computationally-intensive and time-consuming: the large volume of data acquired from environmental biofilm samples (number of DNA reads and MS/MS spectra acquired) and the diverse species complexity present in the environmental sample. To address these challenges, we constructed the metaproteome data analysis pipeline using open-source applications featuring use of the message-passing interface (MPI) for parallel computing. At present, the pipeline features open-source applications Omega, for assembly of DNA segments, Prodigal for prediction of open-reading frames, and the Sipros programs for protein identification.

Results: In FY16, computational resources were used for analyses of large-scale data tiers, resulting in 1 peer-reviewed publication and 4 conference proceedings. One of the seven FY15 publications, a description of protein identifications of a microbial fuel cell (MFC) biocathode, received an ARPAD publication award in March 2016. The genome sequence of *Larbenzia* sp.CP4, an isolate from the MFC biocathode, was reported in FY16, which leveraged HPC resources for genome assembly. Acquisition of qualitative and quantitative proteome profiles of another microbe isolated from the MFC biocathode, *Marinobacter* sp. CP1A, was also described leveraging HPC resources for protein identification and functional inference from sequence homology to well-characterized proteins. Collectively, these results highlight utility of HPC resources in bioinformatics, specifically for conversion of raw DNA sequences isolated from environmental biofilms to large-scale protein metaproteome inventories.

DoD Impact/Significance: Application of the metaproteomic data analysis pipeline enables molecular-level characterization of environmental biofilms, which are of DoD/Naval significance for biosensing, alternative energy, and synthetic biology applications. Use of HPC resources has allowed NRL scientists to complete first-in-kind studies, such as those of the MFC biocathode, which represents several genetically-tractable species to harness for synthetic biological purposes, such as alternative energy sources.

Title: Calculation of Materials Properties via Density Functional Theory and Its Extension
Author(s): M.J. Mehl
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: Cray XC40 [ARL, MD]; Cray XE6 [ERDC, MS]; Cray XC30, SGI ICE X [AFRL, OH]

Research Objectives: The determination of materials properties from accurate first-principles density functional theory (DFT) computations is limited by the small systems sizes, on the order of one hundred atoms, which can be fit onto modern computers. Even order of magnitude improvements in computational speed will only double the number of atoms in the system. Calculations of properties such as diffusion, structure and motion of defects and dislocations, crack propagation and the electronic response of large-scale systems requires system sizes of up to one million atoms. The Center for Computational Materials Science has developed a variety of algorithms grounded in DFT and extended to handle all of these types of calculations. This project will use the techniques to study the properties mentioned above as well as other properties of materials of interest to the Navy.

Methodology: Electronic structure calculations, using the virtual crystal approximation.

Results: We have show that substitutions of Phosphorus and Chlorine for Sulfur can increase the superconducting temperature in the new high-pressure, high-temperature superconductor H_3S.

First principles calculations for the band structure of $CsPbX_3$, where X = Cl, Br, and I, have been carried out as part of the investigation of these materials in nano-scale photovoltaic devices. Standard density functional theory calculations severely underestimate the band gap of these systems. Even hybrid functional calculations only reach a band gap of about 1.5 eV for $CsPbBr_3$, though the experimental band gap is about 2.6 eV, so a scissors operator will have to be added to these results. Analysis of the effect of the band structure on the photovoltaic properties of these materials is underway.

First principles calculations have been started to determine second and third-order force constants for various structures in the Ga_2O_3 system, as a test of the ability of Density Functional Theory to predict thermal conductivity. The force constants for beta Ga_2O_3 have been calculated, and analysis is underway to determine the thermal conductivity.

Future plans: We will continue to investigate the $CsPbX_3$ system, especially trying to determine if any modification of Density Functional Theory (GW, LDA+U, hybrid functional, etc.) can reproduce the experimental band gap.

DoD Impact/Significance: The epsilon phase of Ga_2O_3 is of interest because of its thermal conductivity. Unfortunately this material has many vacancies on the Ga sites. We will study a variety of structures for this phase, find the second- and third-order thermal conductivity for the lower energy structures, and do an ensemble average to determine the approximate thermal conductivity of epsilon Ga_2O_3.

Title: Quantum-Chemical Simulation of Surface-Science Experiments
Author(s): V.M. Bermudez
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

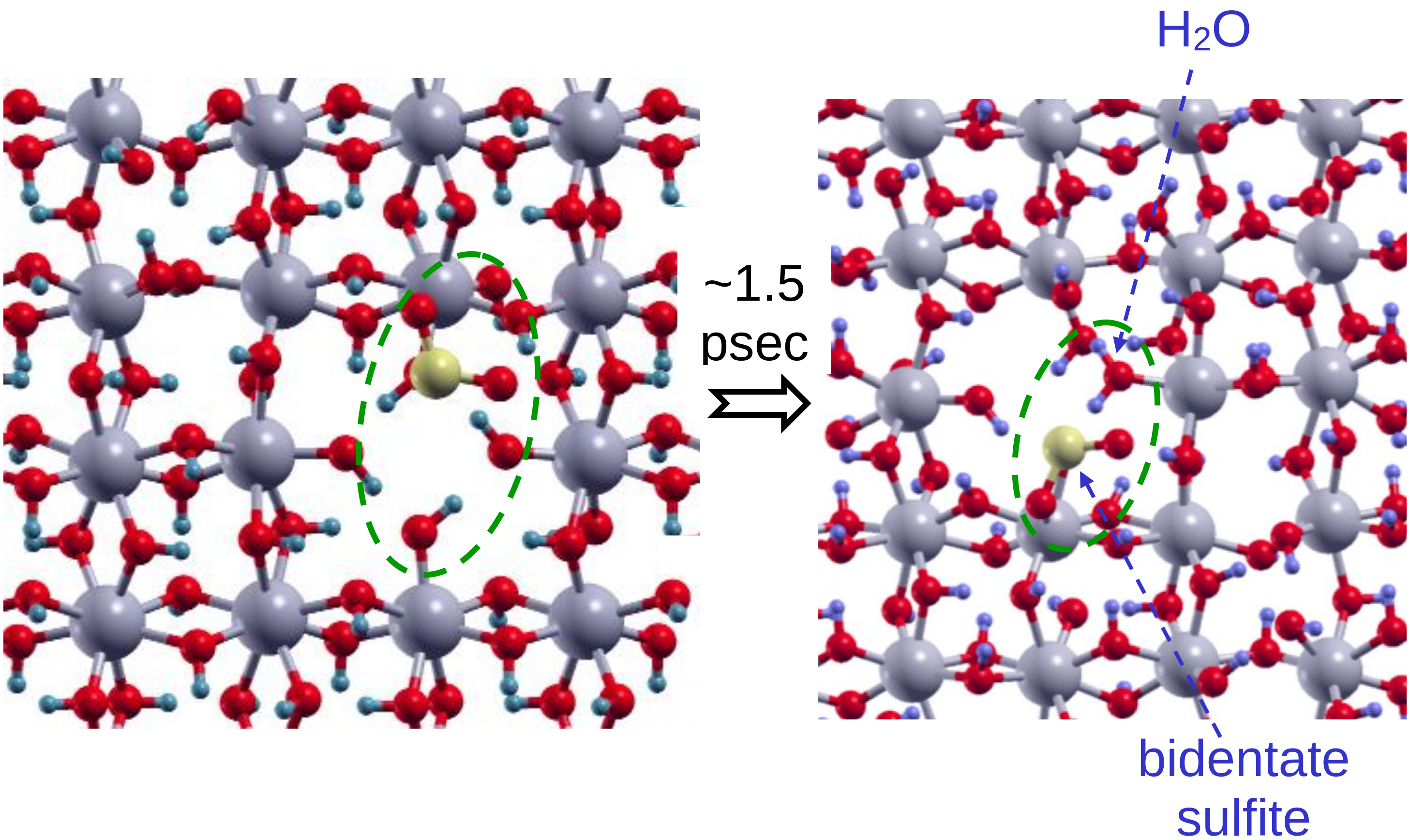
Computer Resources: SGI ICE X, Cray XC30 [AFRL, OH]; SGI Altix ICE [NRL, DC]

Research Objectives: The objective of this program is to perform quantum-chemical calculations as an aid in interpreting surface-science experiments and in predicting gas-solid interaction.

Methodology: The QUANTUM ESPRESSO 5.0 and 5.1 software packages are used for density functional theory (DFT) calculations on periodic structures. The GAUSSIAN 09 software package is used for DFT calculations on isolated molecules and clusters.

Results: The removal of toxic substances from air is a subject of great importance with both military and civilian applications. Recent work at the Army's Edgewood Chemical and Biological Center (ECBC) has revealed that $Zr(OH)_4$ is potentially valuable in this area and can be significantly more effective than traditional adsorbent materials such as activated charcoal. $Zr(OH)_4$ has a high density of hydroxyl (OH) groups with both acidic and basic character. The acidic sites exist as OH groups that form bridges between adjacent Zr sites, while terminal groups (OH bonded to a single Zr) exhibit basic character. $Zr(OH)_4$ is commercially available in the form of high-surface-area powders. It is the combination of high surface area and high density of OH groups having both acidic and basic character that makes this material potentially effective in trapping and retaining a wide range of different toxic agents. At present, the physical and chemical structure and properties of $Zr(OH)_4$ are poorly understood. This has led to a basic-research effort, supported by the Defense Threat Reduction Agency (DTRA), that is aimed at characterizing this material and at developing a microscopic, bond-specific understanding of how it interacts with toxic agents. One such species is sulfur dioxide (SO_2), the interaction of which with $Zr(OH)_4$ has been studied experimentally by ECBC. The data suggest that SO_2 reacts primarily with basic (terminal) OH groups to form a bidentate sulfite (SO_3) species with two Zr-O-S bonds to a single Zr, as shown in Fig. 1; however, the mechanism of the reaction remained unknown. *Ab initio* molecular dynamics (AIMD) has been used to simulate the reaction. The results support the previous qualitative interpretation by showing that terminal OH groups are indeed the reactive sites and that bidentate sulfite is the product. The calculation also shows the reaction is a concerted process wherein H is transferred from one Zr-OH to another to form adsorbed H_2O. The dangling Zr-O bond thus formed then reacts with SO_2 to form SO_3, and the process is exothermic by 29.7 Kcal/mol. The activation energy barrier for the reaction is 6.2 Kcal/mol. Work is presently in progress, in collaboration with ECBC, to extend this effort both experimentally and computationally to other toxic agents and to simulants for these agents.

DoD Impact/Significance: These results constitute the first attempt to model quantitatively the reaction between $Zr(OH)_4$ and a representative toxic species. The good agreement between theory and experiment appears to validate the computational approach, and the insight gained into the reaction mechanism indicates that results for other agents and simulants will be useful in developing this material for practical air purification.



$$\text{Zr-OH} + SO_2 + \text{HO-Zr} \rightarrow \text{Zr(-O-)}_2\text{SO} + H_2O\text{-Zr} + \Delta E = 29.7 \text{ Kcal/mol}$$

Figure 1. Results of an *ab initio* MD calculation for the reaction of SO_2 with $Zr(OH)_4$. The left-hand panel shows the $Zr(OH)_4$ supercell formed from a 4x4 polymer of single $Zr(OH)_4$ units linked by Zr-O(H)-Zr bridges. One of the 16 units is removed to make a "defective" structure with terminal OH groups. An SO_2 molecule is placed above the vacancy at the start of the MD run. The right-hand panel shows the reaction product that forms after about 1.5 psec (0.25 fsec time step) at a simulation temperature of 200 K. The reaction sequence below shows the mechanism, which involves transfer of an H to an OH site, to make H_2O, coupled with the formation of bidentate sulfite (SO_3). The reaction is exothermic by 29.7 Kcal/mol. Gray, red, yellow and blue spheres are Zr, O, S and H respectively.

Title: *Ab initio* Modeling of Graphene Hot Electron Transistors
Author(s): J.G. Champlain and B.D. Kong
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: SGI ICE X [AFRL, OH]; Cray XE6 [ERDC, MS]

Research Objectives: The goal of this study is to predict and understand the electrical properties of future graphene devices. Especially, the physical properties and charge transport characteristics of various graphene interfaces are the main subject of the study. Density functional theory (DFT) is used to form a complete understanding of the graphene interfaces with various materials in order to support the on-going experimental efforts. This study will provide fundamental level understanding on heterogeneous graphene systems and guiding information for future experiments and analysis at NRL.

Methodology: DFT atomic structure calculation is used to analyze electronic and vibrational properties of heterogeneous graphene-semiconductor interfaces.

Results: Surface fluorinated monolayer and bilayer graphene sheets have been analyzed using Quantum Espresso DFT package. The optimized atomic configurations which were obtained by minimizing the interatomic potential were found for each structure. The resulting electronic structure suggests that the surface fluorination is an excellent way of converting the graphene to the thinnest insulating barrier that can be used as tunneling barrier for a graphene base hot electron transistor. It is also found that the surface fluorination of bilayer graphene results in a unique insulator-semiconductor heterogeneous structure. The graphene exposed to the fluorine becomes wide bandgap insulator and dipole induced by the fluorinated graphene creates a band gap on the adjacent graphene layer, converting it into semiconducting. In addition to the DFT studies, the scattering rates of electrons traveling across graphene sheets has been also studied.

DoD Impact/Significance: Graphene has drawn significant amount of interests from scientific communities not only because of their peculiar electrical and mechanical properties stem from the two dimensional nature but also because of the potential great impact on future electronic applications. Graphene base hot electron transistors are one of the most promising candidates which could enable novel high frequency and high power electronic devices. The electronic properties of a few atom thick graphene layers sandwiched between two wide bandgap materials is important information in fabricating and optimizing such devices. The estimated physical characteristics of graphene in the realistic environment can work as a valuable guidelines to expedite the realization of the proposed devices.

Title: Preventing Corrosion by Controlling Cathodic Reaction Kinetics
Author(s): S. Policastro[1] and J. Keith[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]Univeristy of Pittsburgh, Pittsburgh, PA
CTA: CCM

Computer Resources: SGI Altix ICE [NRL, DC]

Research Objectives: The goal of this project is to determine the effect of dopant elements on the kinetics of oxygen reduction reaction catalyzed on titanium oxide in order to develop new approaches for controlling galvanic corrosion between fastener and structural aircraft alloys.

Methodology: We created a model amorphous TiO_2 surface by annealing a rutile 100 slab at 1000 K using ReaxFF as employed in LAMMPS. We used the force field created by Kim et. al. (DOI: 10.1021/la4006983) as it is specifically parameterized to model bulk TiO_2. We tested various slab sizes by varying the number of primitive unit cells along the x and y axes in the original rutile 100 slab. The Ti-Ti pair radial distribution function approximately converged by the 3x3 unit cell slab. We then relaxed the ReaxFF annealed structures using the Vienna ab initio Simulation Package (VASP). These calculations used the PBE exchange correlation functional, PAW psuedopotentials, energy cut offs of 450 eV, and a 2x2x1 kpoint grid. We found that these energy cutoffs and kpoint grids gave well converged oxygen vacancy formation energies. The VASP relaxed structure has Ti-Ti, Ti-O, and O-O radial distribution functions that match experimental RDF data more closely than the ReaxFF annealed structures. As such, this surface is a suitable model for a real amorphous TiO_2 surface.

Results: Our prediction that Co, Sn, and Cr will have lower ORR activity than pure TiO_2 is consistent with the previous experimental report. Fine tuning our model to predict the correct relative magnitude of the decrease in ORR activity would require future work to analyze the impact of each elementary reaction step on the overall ORR process. Currently, we predict that any dopant that destabilizes the intermediates ($\Delta G_{*OH} > 1$ eV) will hinder ORR kinetics. While we also believe that certain dopants with $\Delta G_{*OH} < 1$ eV can reduce ORR reaction rates (V, Sn, Cr, Mo) more work is required to completely understand the impact of these dopants.

DoD Impact/Significance: The predictions of the effect of dopant atoms on ORR kinetics has been used to cast binary Ti alloys that have then been experimentally tested to confirm the suppressed ORR kinetics. We intend to transition these approaches to the development of fasteners used in Naval ariframes.

Title: Magnetic Materials and Heterostructures
Author(s): K.M. Bussmann
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CCM

Computer Resources: Cray XC30 [AFRL, OH]

Research Objectives: Perform *ab initio* electron-structure calculations of magnetic materials to determine how magnetic properties are modified in response to electron charge dosing and strain. In particular, determine the behavior of the magneto-crystalline anisotropy of uniaxial magnetic materials and the wave-vector modulation of non-collinear magnetic materials in response to changes in local electron charge density or changes in crystal lattice dimension.

Methodology: The Full Potential-Linearized Augmented Plane Wave + local-orbital (FP-LAPW+lo) method embodied in the 'elk' software package is our primary tool used to evaluate the materials of interest. We make use of the built-in capability to determine the ground state energy of magnetic materials in response to variations of spin-orbit coupling, spin-spiral, charge dosing, and strain parameters. FePd, FePt and $SmCo_5$ are three magnetic compounds being studied for the modulation of uniaxial magneto-crystalline anisotropy. Tetragonal $MnAu_2$ and hexagonal Dy are the primary focus of non-collinear magnetism studies for the helical spin ordered state.

Results: The compound $MnAu_2$ has tetragonal symmetry composed of layers of Mn separated by 2 layers of Au propagating in the c-axis direction. Mn retains a local magnetic moment and displays ferromagnetic order within each Mn plane. Glasbrenner et al. [1] have shown the competition of the interlayer anti-ferromagnetic super-exchange and ferromagnetic Mn-Au s-d exchange interactions cause the lowest magnetic ground state to form a spin-spiral with magnetization direction within the Mn a-b plane but with direction rotating ~ 45 degrees from layer to layer along the [001] direction. The resulting spin-spiral magnetic order has been experimentally shown to persist to T ~ 360K. HPCMP computations using the elk code have demonstrated the modulation of the spin-spiral wave-vector with electrical charge. The ground state spiral wave-vector was determined for a range of charge affected by electric-field gating of $MnAu_2$ atop an insulating dielectric layer. The application of -0.03 electrons of charge per unit cell – a value that is experimentally feasible – is sufficient to cause the ground state order to change from 45 to 90 degrees rotation per Mn layer. A conceptual device making use of an overlayer magnetic free layer that can be incorporated to a magnetic tunnel junction to provide electrical readout of the orientation that would allow use in integrated, non-volatile information storage.

DoD Impact/Significance: These results provide theoretical impetus to pursue experimental work to establish the use of non-collinear magnetic materials for ultra-low power and non-volatile information storage. The proposed device utilizes electrical field and associated charge modulation at a dielectric-metal interface to control magnetization direction and removes the need for current-driven control such as is presently used in spin-transfer torque magnetic random access memory (STT-MRAM). These results, if proven experimentally, will open a new avenue for ultra-low power information processing.

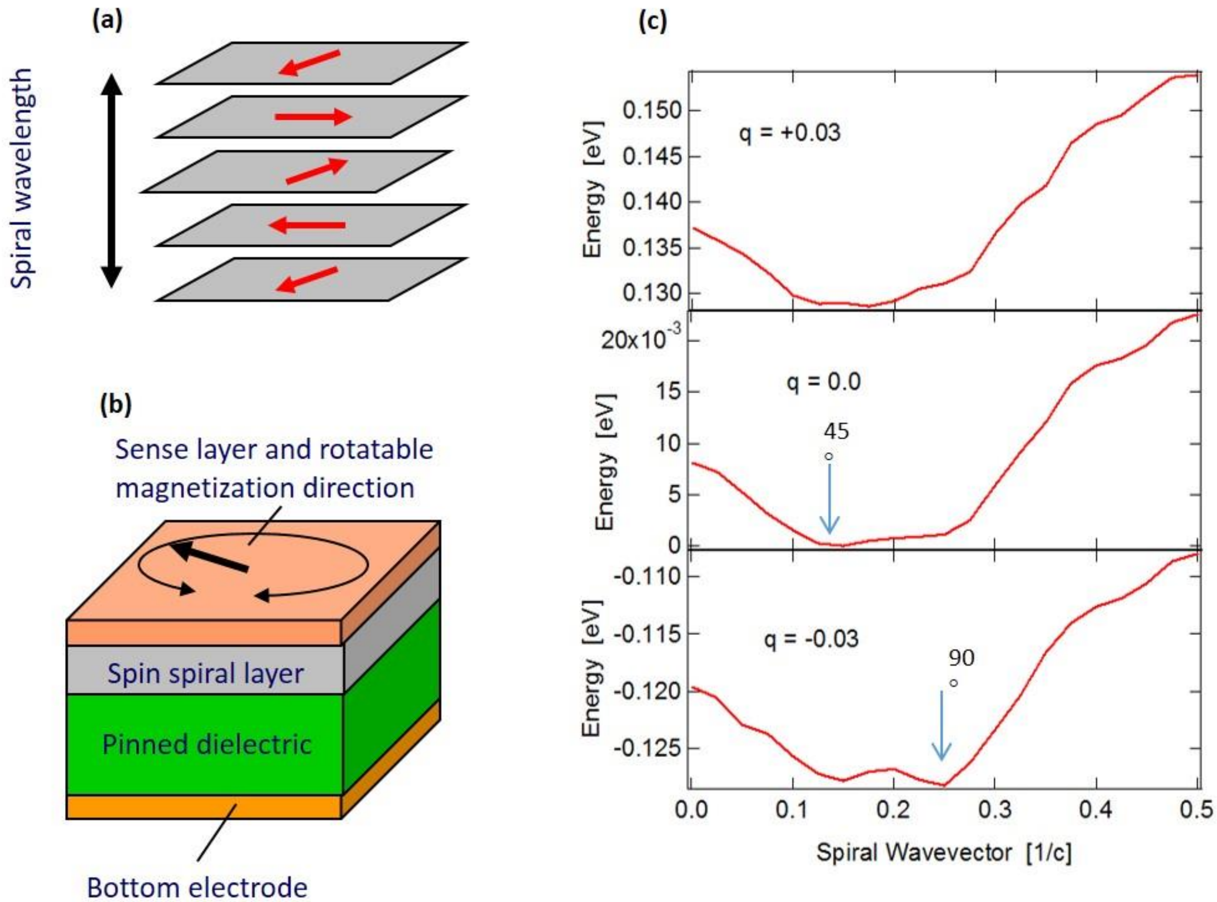


Figure 1. Magnetic layers showing a spin-spiral magnetic order as in $MnAu_2$ (a), a conceptual device showing charge-modulation by use of pinned dielectric layer gate (b), and the ground state energy of $MnAu_2$ as a function of charge dosing of the unit cell and spin-spiral wave-vector (c).

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CEA

Computational Electromagnetics and Acoustics

CEA covers two primary computational disciplines: electromagnetics and acoustics. Computational Electromagnetics covers the high-resolution multidimensional solutions of Maxwell's equations. DoD applications include calculating radiofrequency sensor performance; radar scattering of tactical ground, air, and sea vehicles; the electromagnetic signature of buried munitions; high-power microwave performance; and the interdisciplinary applications in magnetohydrodynamics and laser systems. The Computational Acoustics area covers the high-resolution multidimensional solutions of the acoustic wave equations in solids, fluids, and gases. DoD applications include the modeling of acoustic fields for surveillance and communication, seismic fields for mine detection, and the acoustic shock waves of explosions for antipersonnel weapons.

Title: Small Slope Approximation Rough Surface Back-Scattering Analysis
Author(s): J. Alatishe
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: SGI ICE X [AFRL, OH]; Cray XE6 [ERDC, MS]; SGI Altix ICE, Exxact HD GPU Cluster [NRL, DC]

Research Objectives: The objective of this project is to determine and characterize the spatial coherence effects that are inherent in sea clutter by numerically analyzing the associated response at the antenna port of a monostatic radar. The sea surface coherence effects are examined with respect to the associated antenna characteristics and the surface properties.

Methodology: The surface model used is based on empirical data as represented by the ocean wave-number spectrum for a fully developed sea, from which statistical realizations of the ocean surface are generated. Once the response from the surface has been computed, the properties of the simulated sea-clutter responses are characterized. The Scattering Amplitude (SA) of the surface characterizes the spatial coherence. Once the SA has been computed, the response at the antenna port is determined and the coherence effects due to the surface are examined. Numerical integration was used to determine the antenna response from the rough surface profile. The SA has a nonlinear relationship with the surface profile, which is evaluated by the Fourier Transform of a linearized sea surface model that employs the ocean wave-number spectrum. The ocean wave-number spectra were represented by the Elfouhaily ocean wave-number spectrum at different ranges of wind speeds and wind directions. With the SA and surface model calculated, the response at the antenna port was computed for a given antenna aspect angle. The codes that were used to execute these steps were first written in MATLAB and then converted into FORTRAN 90. Then the codes were parallelized using the Message Passing Interface (MPI) and run on 1024 processors or up to eight graphics processing units (GPUs) at the HPC facility. Multiple simulations were conducted for similar surface conditions at X-Band (10 GHz).

Results: Data obtained from published accounts of sea clutter were used as the baseline for comparison. These sea-clutter values were measured at various wind speeds and wind directions for given antenna aspect angles (elevation and azimuth) and polarizations of the antennas. The simulated received sea-clutter responses were computed for different elevation angles for vertical and horizontal polarizations. The simulation generated the frequency response of the sea surface for a given sea state for an observed time increment. The FFT fast convolution was used to generate the complex time-dependent echo from the spectral product of the frequency response associated with the sea surface and the transmitted waveform. As a result of the previous step, multiple coherent processing intervals (CPI) were generated for analysis. The simulation results showed that the range-Doppler properties are similar to real sea clutter, but not completely accurate due to the lack of the non-linearities in the surface model. However, sea-spike phenomena are present in the simulated data and the statistics of the clutter appears to closely match that of real data. More investigation of the simulated data is still required.

DoD Impact/Significance: Examining the spatial coherence effects in radar sea clutter will provide further insight into the phenomenology of back scattering from the ocean, which will be useful in devising algorithms for detecting threats over the sea.

Example results:

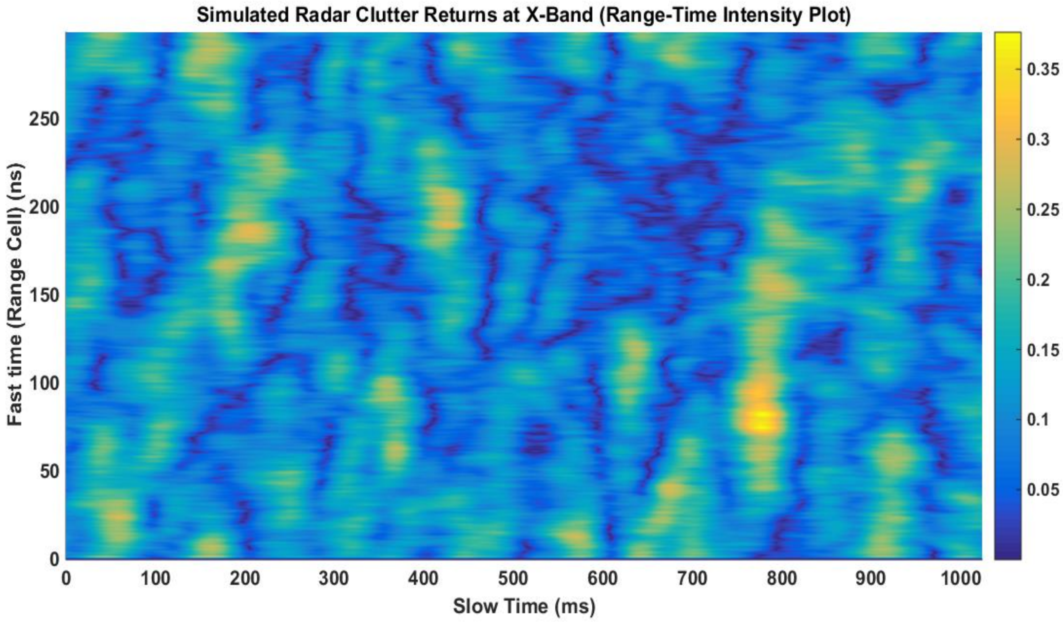


Figure 1. Range-Time Intensity plot of X-Band sea-clutter returns for HH polarization at 65^o elevation. Pulsewidth is 100ns, pulse repetition interval is 200 ms, and wind speed is 10 m/s at crosswind

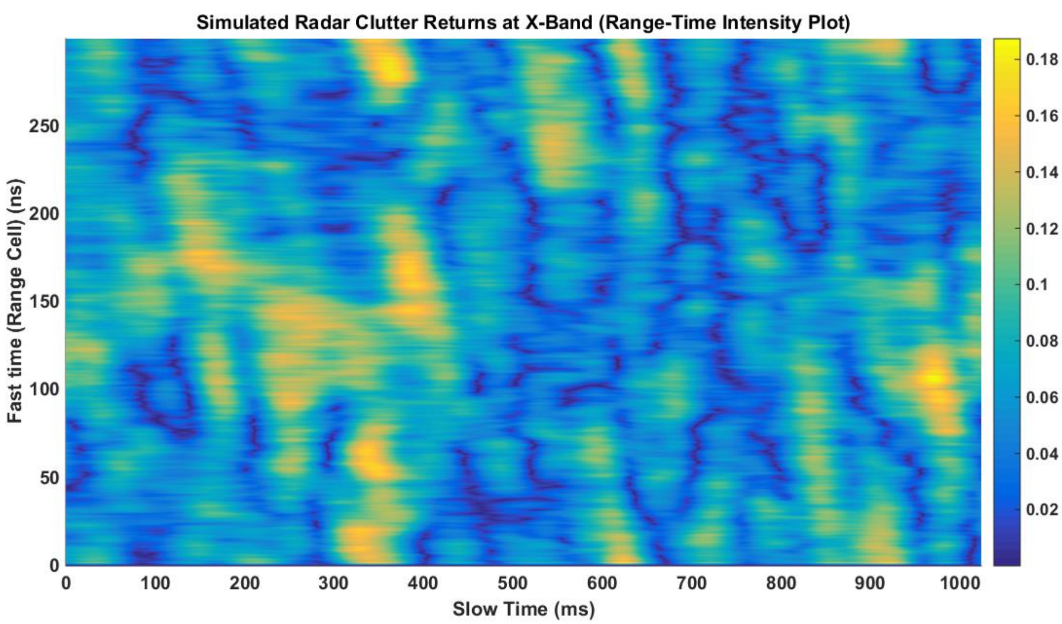


Figure 2. Range-Time Intensity plot of X-Band sea-clutter returns for VV polarization at 65^o elevation. Pulsewidth is 100ns, pulse repetition interval is 200 ms, and wind speed is 10 m/s at crosswind

Title: Optomechanical Systems
Author(s): M. Zalalutdinov, S. Carter, and S. Dey
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: Cray XC40 [ARL, MD]; SGI Altix ICE [NRL, DC]; Cray XE6 [ERDC, MS; SGI ICE X [AFRL, OH]

Research Objectives: Study of the dynamic response and stress distribution in high frequency nanomechanical resonators nested with optical cavities. The objective is to design a low loss (high quality factor) mechanical structures with normal modes featuring a highly inhomogeneous spatial stress distribution, with areas of high stress concentration.

Methodology: We use a high-order finite element based approach to simulate the dynamics of photonic crystals both for natural modes of vibration as well as due to applied excitation.

Results: In Fig. 1, we illustrate the volumetric strain patterns corresponding to different normal modes for tuning-fork-type structures.

DoD Impact/Significance: The design will be used for a new class of optomechanical systems with quantum dots embedded in the mechanical structures and used as a local optical readout for time-variable local strain with high-level of sensitivity.

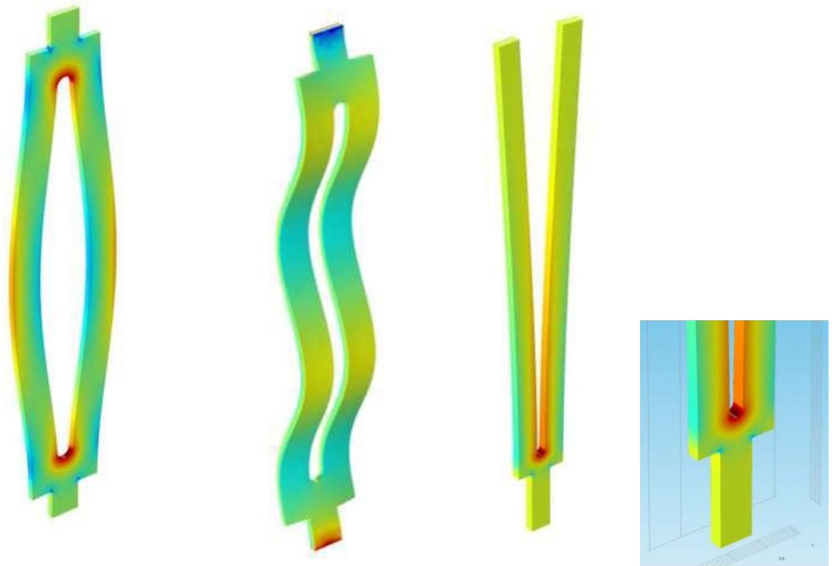


Figure 1. Dynamics response modes and stresses for various tuning-fork shapes.

Title: Forward Simulations of Diffusive Wave Algorithms (Replaces Terahertz Acoustics)
Author(s): D. Photiadis
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: Cray XC40 [ARL, MD]

Research Objectives: Develop forward numerical simulation models in disordered, acoustic media which can be used to test and further develop diffusive wave based detection algorithms.

Methodology: (1) Brute force 2D PE with "random sound speed fluctuations." (2) Full wave numerical solution of wave equation in "toy model."

Results: Initial results. Approach 1: Insufficient randomness to produce saturation, no backscattering, conventional imaging is sufficient. No diffusive regime so one cannot evaluate a diffusive wave algorithm. Research in this direction is ongoing. Approach 2: Simulations successfully model diffusive behavior in a uniform medium (refractive medium is no more difficult). Conventional imaging fails while the diffusive wave algorithm appears to be successful. This behavior is shown below in Fig. 1 for a numerical simulation in a disordered medium. The simulation is fully 3-dimensional despite the fact that only the *x* and *z* axes are shown in the figure. Hot colors (red, yellow…) indicate a possible detection. The actual target in the simulation is shown as the red solid ellipse. While conventional imaging does show some response near the position of the actual target, substantial "noise" is also evident and thus no detection can be inferred. The diffusive wave algorithm successfully filters out this "noise."

DoD Impact/Significance:

- The diffusive wave algorithms have the potential to significantly increase our range/environment of detection for ASW, UUV and mines.
- The results of this effort will be used to design an upcoming (summer 2018) at-sea experiment.
- Possible enhancement of SURTASS-LFA performance for ASW.
- These simulation results testing the diffusive wave algorithm will be the first such reported numerical simulations.

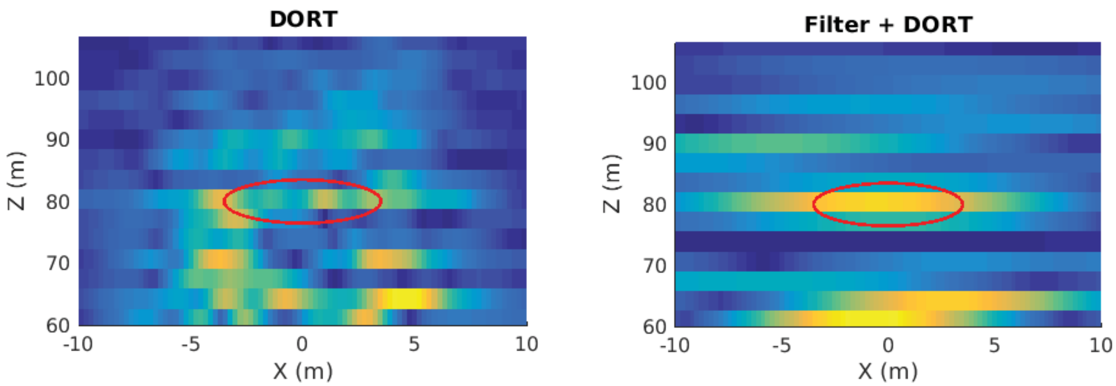


Figure 1. Target detection with diffusive wave processing compared to DORT (conventional) imaging.

Title: Low Grazing Angle Radar Backscatter
Authors: J.V. Toporkov and M.A. Sletten
Affiliation: Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: IBM iDataPlex [MHPCC, HI]; SGI UV2, Cray XC30 [AFRL, OH]; Cray XE6 [ERDC, MS]; Cray XC40 [ARL, MD]

Research Objectives: Backscatter from sea surface is routinely present in coastal and ship-borne radar systems, many operating in low grazing angle (LGA) regime. It is often regarded as clutter that masks a target echo, but also can be a source of information about ocean environment. Good understanding of the properties of surface backscatter, their dependence on environmental parameters, and their distinctions from those of man-made target echoes are key to improving or even enabling performance of such radar systems and applications. This project investigates detailed characteristics of radar returns from ocean surface with possible presence of embedded targets. The task is accomplished through simulations that involve both direct numerical solution of the scattering problem and, where appropriate, numerical implementations of approximate scattering models.

Methodology: The approach combines physics-based models for ocean surface and floating targets evolution with computationally efficient, exact evaluation of the electromagnetic backscatter. A wind-driven surface is represented by realizations of a Gaussian random process defined by the Elfouhaily wave spectrum. Interactions between surface harmonics affecting shape and motion of the small-scale roughness (that has great impact on scattering of centimeter-scale electromagnetic waves), are modeled by the Creamer transformation applied to the Gaussian realization. Motion of a semi-submerged round target is deemed to be defined by the orbital wave current (derivable from the known surface profiles) at the location of its center. The electromagnetic field scattered by a “time-frozen” scene (surface with the broached part of the target) at a particular frequency is found by iteratively solving a boundary integral equation for the induced surface current. The formulation is based on first principles and automatically accounts for many phenomena (multiple scattering, shadowing) known to be problematic for analytical treatment. The calculations are conducted at a number of frequencies, and Fourier synthesis is used to simulate pulse scattering. The procedure is repeated for every “surface+target” profile in the sequence representing temporal evolution. The simulations are limited to the two-dimensional space but have direct relevance to commonly occurring three-dimensional geometries (e.g., incoming long-crested waves).

Results: Simulations were conducted for X-band signals using the setup shown in Fig. 1. The scene contained three floating round objects of various sizes. The 20 s-long data records were generated for wind speeds of 5, 7 and 10 m/s and the incidence angles θ_i within the range 20-87 degrees. The covered frequency band of 1.25 GHz allowed producing surface echoes corresponding to pulses as short as 2.3 ns (or 0.34 m). Figure 2 shows such a record at $\theta_i = 70°$. The target signatures are visible against the ambient clutter, especially at the horizontal transmit/receive (HH) polarization. Figure 3(a) displays the Doppler spectrogram evaluated for the complex data transect at the ground range of 34.5 m (cf. Fig. 2) using a 0.5 s-wide sliding Hann window. The simulations can be repeated for the same surface profile in the absence of the target allowing a uniquely precise comparison to the spectrogram of the surface clutter shown in Fig. 3b. The dissimilarities, especially in the width and locations of spectral maxima can be exploited to differentiate the target from the ambient clutter. The simulated data were supplied to the Radar Division for further analysis and use.

DoD Impact/Significance: Detection of low-observable targets on the sea surface is a quintessential Navy problem. As radar systems adopt broader capabilities (polarization, Doppler), new sets of properties of the sea and target backscatter come to attention. When properly investigated and understood, dissimilarities in these characteristics can become the basis for advanced target detection algorithms.

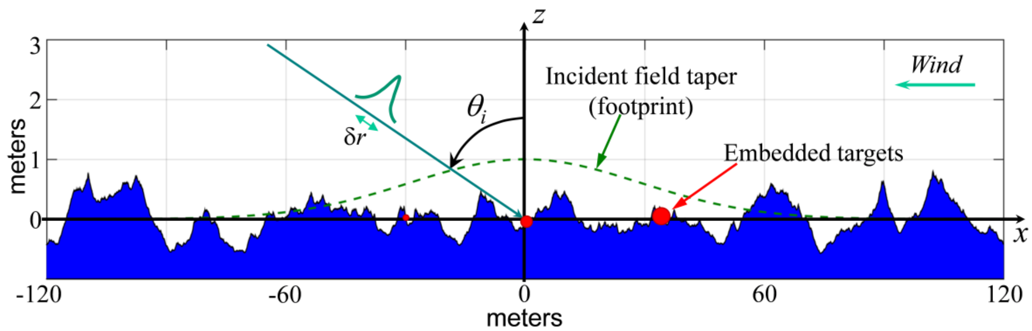


Figure 1. Setup for scattering simulations from evolving surface with floating bodies.

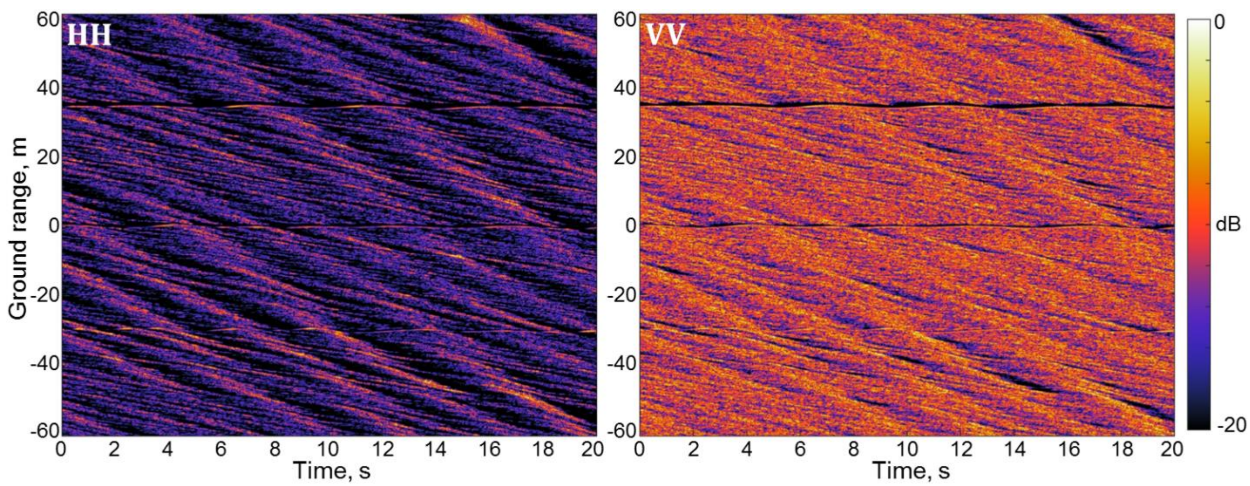


Figure 2. Intensity (in time-range format) of simulated echoes from evolving surface with 3 floating round bodies. Incidence angle θ_i is 70°, the surface corresponds to 7-m/s wind speed, and resolution is 0.34 m.

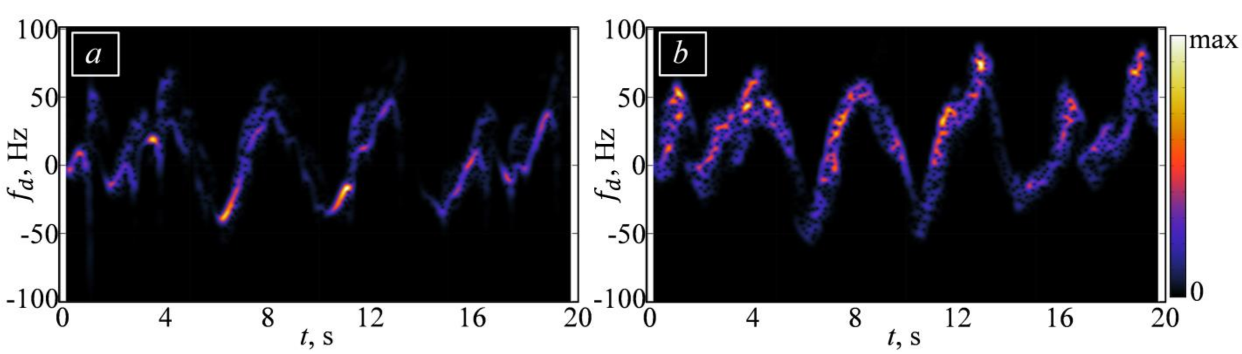


Figure 3. Magnitudes of the HH-polarized Doppler spectrograms evaluated along the constant-range transect x_g = 34.5 m (cf. Fig. 2(a)) with a sliding time window. a) Target present; b) target absent (sea surface only). Linear scale, with each plot normalized to its own maximum. Wind speed is 7 m/s, θ_i = 70°. and resolution is 1.0 m.

Title: Intense Laser Physics and Advanced Radiation Sources
Author(s): D.F. Gordon,[1] L. Johnson,[1] B. Hafizi,[1] M. Helle,[1] Y. Chen,[2] J. Palastro,[1] and J. Penano[1]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]RSI Inc., Lanham, MD
CTA: CEA

Computer Resources: Cray XE6, SGI ICE X [ERDC, MS]; Cray XC30 [AFRL, OH]

Research Objectives: The primary objectives of this program are to model the propagation of intense, short-pulse lasers in plasmas and other nonlinear media, and to provide computational support for experiments on the NRL Terawatt-Femtosecond-Laser (TFL). Current areas of research include plasma based accelerators, novel sources of short pulse infrared radiation, ultra-high field physics, and hypersonic flow modeling.

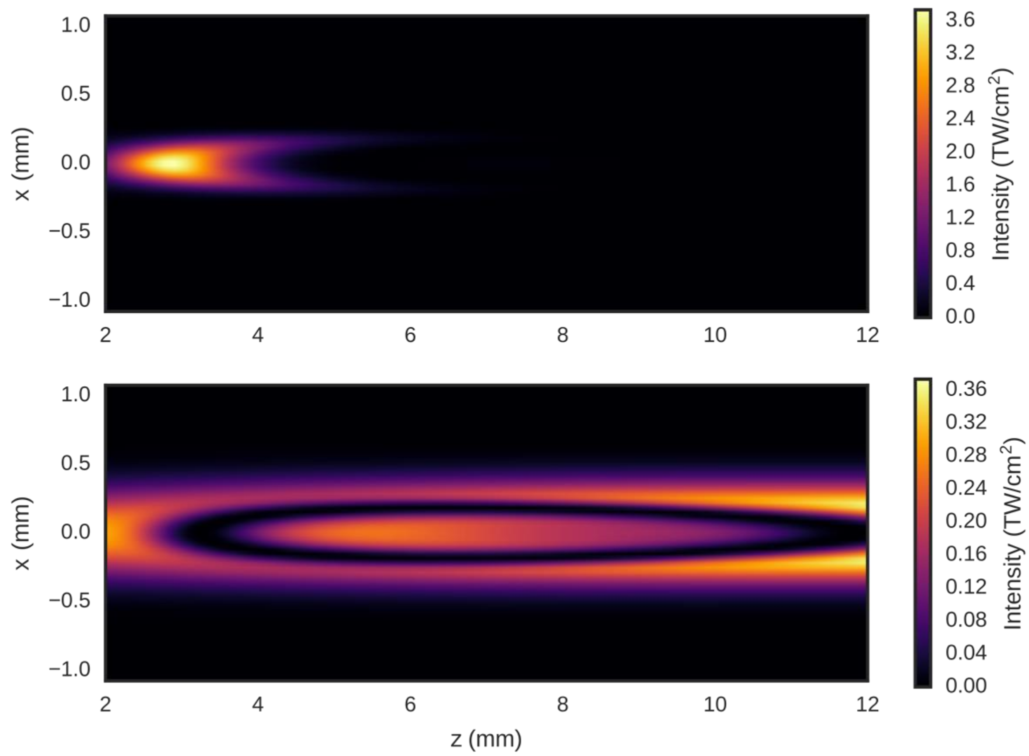
Methodology: HPC resources are utilized using an object oriented parallel framework called turboWAVE, which contains modules designed to solve a variety of problems. Both fully explicit and ponderomotive guiding center particle-in-cell (PIC) modules are used to model relativistically intense laser pulses propagating in plasmas. Quantum optics modules are used to describe the interaction of the laser pulse with atoms or ions. Fluid modules are used to describe hypersonic flow and shock propagation in gas targets. The framework universally supports distributed memory parallelization via the Message Passing Interface (MPI). Some modules support general purpose graphical processing units (GPGPU) via OpenCL.

Results: Simulations were carried out of short-pulse (~1 picosecond) long wavelength (~10 micron) radiation generation by means of backward Raman amplification (BRA). Generally, most efforts in BRA are focused on near-infrared radiation. This research investigates whether BRA is useful for amplifying and compressing longer wavelength pulses. An important objective is to discover a means of generating terawatt-class mid-to-long infrared radiation using techniques that are scalable to high repetition rate. The simulations use both fluid and PIC models, with the fluid model being useful due to its ability to treat collisions, and the PIC model being useful due to its ability to treat higher intensity regimes. The compression and amplification process was calculated to produce high irradiance long wavelength radiation using a carbon dioxide laser as a pump source. An example of a two-dimensional fluid simulation is shown in the figure.

We carried out a parameter scan in three dimensions in order to benchmark relativistic tunneling ionization theories. Absolute ionization rates are difficult to measure experimentally, so that competing theories are difficult to assess. Ab initio simulations, up until now, have been criticized as not properly accounting for relativistic effects. Our three dimensional simulations utilizing HPC resources answer this criticism. We determined that the theories over-estimate the rate by a factor of several in some parameter regimes, and discovered an interesting relationship between the timing of the ionization current and the applied electric field.

We extended the turboWAVE quantum optics module to treat spin ½ particles by direct solution of the time dependent Dirac equation. An algorithm was devised that effectively utilizes multiple levels of parallelism, through combined OpenCL and MPI programming. The algorithm was validated by closely reproducing the relativistic Zeeman splitting results from a separate time independent algorithm, and by comparison with analytical solutions where possible. Preliminary tunneling ionization runs were carried out with a particular spin orientation.

DoD Impact/Significance: Laser-driven accelerators and radiation sources have potential applications for ultrafast (femtosecond) imaging of chemical and biological systems. High-energy electron beams might be useful as a gamma ray source for detection of special nuclear materials (SNM). High-energy ions might also be useful for SNM detection, or for cancer therapy.



A picosecond, 11.7 micron seed pulse (top) is amplified and compressed by a 10.6 micron pump pulse (bottom) until it has depleted the pump of a significant fraction of its energy. The seed pulse propagates from right to left, the pump pulse from left to right.

Title: Large-Scale Simulation of Traveling Wave Tube Amplifiers
Author(s): G. Stantchev and S. Cooke
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: SGI ICE X [AFRL, OH]; Cray XC30, IBM iDataPlex [NAVY, MS]

Research Objectives: The focus of the project during FY16 has been on continuing the integration of the HPC version of NRL's 3D Electromagnetic PIC Code Neptune with Sandia's DAKOTA toolkit and the Air Force Research Laboratory's Galaxy Simulation builder, and extending its capabilities with high-performance uncertainty quantification and reliability analysis.

Methodology: One of NRL's premier design tools for Vacuum Electronics RF amplifiers is Neptune, a highly efficient GPU-accelerated simulation code, which implements a three-dimensional electromagnetic Finite-Difference Time-Domain (FDTD) algorithm coupled self-consistently with a particle-in-cell (PIC) algorithm to model the interaction of an RF wave with a high-power electron beam. Neptune is capable of handling, with high accuracy, complex geometries and various types of media, such as metals, dielectrics, and permeable materials with their appropriate volumetric and surface losses. Neptune was originally designed to run on a single workstation, however over the past few years it has been successfully integrated with an existing global optimization toolkit and a distributed HPC resource management framework for the purposes of accelerating the process of parametric design optimization for Vacuum Electronic (VE) devices. DAKOTA, a multi-level parallel design toolkit developed by Sandia National Labs, has been used as a back end of Neptune's HPC optimization framework. This has presented an opportunity to leverage DAKOTA's extended capabilities for reliability analysis (RA) and uncertainty quantification (UQ), which are becoming increasingly important as VE devices shrink in size, grow more powerful, and thus tend to be more sensitive to material defects and geometry perturbations.

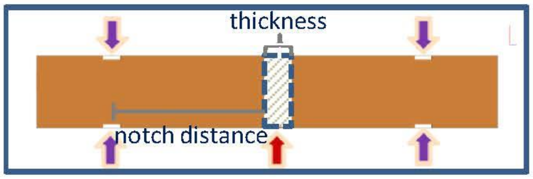
To this end we have studied and evaluated the suite of DAKOTA's RA and UQ algorithms and are in the process of making a select subset available via our integrated HPC deployment framework based on Neptune and AFRL's Galaxy Simulation Builder. Some applicable methods include the Latin Hypercube Sampling and the First/Second Order Reliability Method (FORM/SORM) for performing Most Probable Point (MPP) of failure searches based on a set of user-defined system response levels.

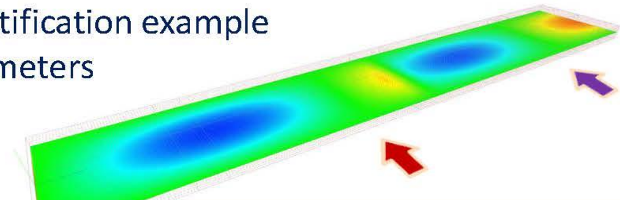
Results: We demonstrated that, in general, local reliability analysis methods perform well in terms of accuracy versus sufficiently dense brute-force sampling, which tends to take orders of magnitude longer to compute. We are currently in the process of performing additional studies to quantify more rigorously the tradeoffs between computational efficiency and accuracy of the various RA and UQ methods for realistic RF amplifier design optimization scenarios.

DoD Impact/Significance: High-power RF amplifiers are critical components of advanced decoys, missile seekers, surveillance radar, electronic warfare systems, communication transmitters, and smart weapons. NRL is the lead DoD laboratory for Vacuum Electronics R&D, developing advanced RF amplifiers to meet Navy/DoD requirements for high peak and average power, high power densities, wide bandwidth, high efficiency, high gain and ease of thermal management. The ability to accelerate and automate the virtual prototyping and optimization of Vacuum Electronics amplifiers, as well as to quantify and analyze the reliability of their components, will ultimately help decrease the time to solution and improve the performance characteristics of these mission-critical RF devices.

Project: Large scale simulation of Traveling Wave Tube Amplifiers

Uncertainty Quantification example
with 2 input parameters

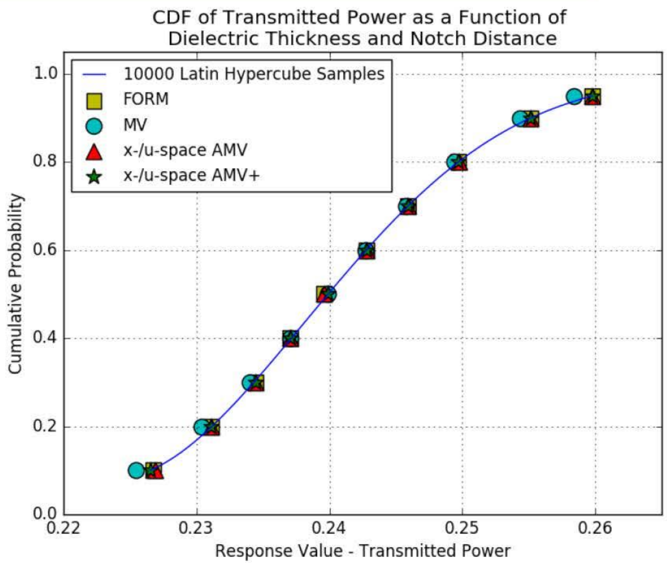


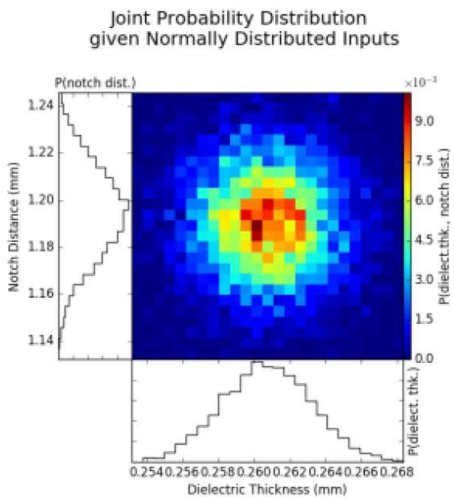


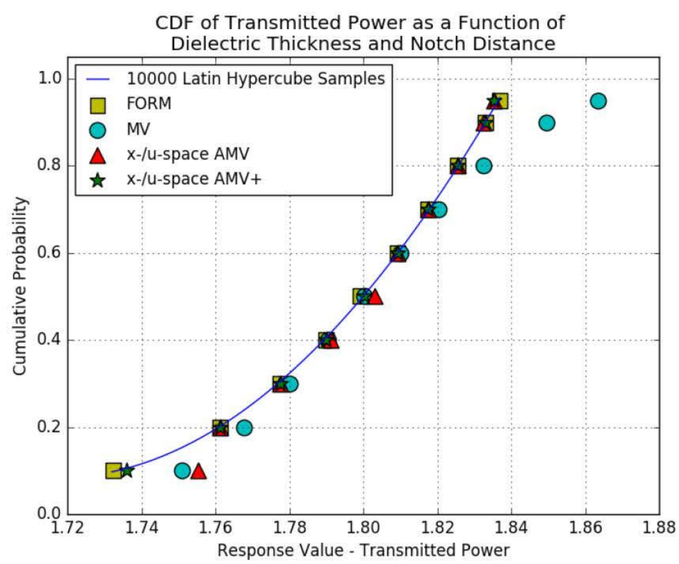
A 3D simulation of a waveguide with a **dielectric window** of varying thickness and symmetrical **notches**

Output: transmitted power for a fixed wideband signal

Optimization parameters, thickness and notch distance, drawn from a Gaussian joint probability density with mean **far from** the local optimal point of the output function







Optimization parameters, thickness and notch distance, drawn from a Gaussian joint probability density with mean **close to** the local optimal point of the output function

Title: Multidimensional Particle-in-Cell Modeling of Ultrashort Pulse Laser with Solid Targets
Author(s): G.M. Petrov
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CEA

Computer Resources: SGI ICE X [ERDC, MS]

Research Objectives: Multidimensional particle-in-cell (PIC) modeling and simulations of the interaction of short pulse laser with micro- and nano-materials for better understanding the dynamics of particle acceleration and X ray and neutron generation.

Methodology: Intense lasers interact with matter in a wide range of time scales. For processes occurring on femtoseconds to picoseconds time scale, adequate description is provided by multidimensional particle-in-cell models. Such models are the primary computational tool for laser-produced plasmas since they provide a self-consistent description of the electromagnetic fields and response of the material. Nowadays, particle-in-cell models are used extensively for modeling laser-matter interaction on micro- and nano-scale. We use a two-dimensional relativistic particle-in-cell code for laser-matter interaction, which was developed in-house at the Plasma Physics Division at NRL.

Results: The particle-in-cell code was extensively used to study particle acceleration and x-ray generation from thin foils and nano-clusters irradiated by ultrashort (fs-ps) high-intensity (10^{19}–10^{22} W/cm^2) laser pulses. The code provided valuable insight into the physical processes occurring during the interaction. It was employed to analyze experiments at the University of California–San Diego, which our collaborators have conducted to further assist in the understanding of target performance in the experiments. In particular, we did a systematic study by varying laser parameters (intensity, duration and focal spot size) and target parameters (material, thickness) in order to quantify particle emission (energy and angular distribution) and optimize targets The model was particularly useful for selecting the right laser systems to conduct very expensive and time consuming experiments by outlining the range of laser and target parameters required for successful generation of high-energy (GeV) directed (<10 degree) heavy ion beams. Using the simulation results as a guidance, experiments were later conducted on the Trident laser at Los Alamos National Laboratory (LANL) and the Texas Petawatt Laser in Austin, Texas. The particle-in-cell code's capabilities were augmented by coupling to an atomic physics code to look into the charge distribution of heavy ions such as gold.

DoD Impact/Significance: This modeling and the results are of significant interest to the Navy and DoD as they are directly related to problems such as generation of X rays and gamma rays, as well as directed particle beams (neutrons, protons, radioactive ion beams), all of which can be used for both fundamental research and practical applications such as detection of nuclear materials and improvised explosive devices. The research is also of great interest to the scientific community dealing with high-energy density plasmas, laser nuclear physics and laser-matter interactions. The simulations have been used to guide experiments related to laser-matter interaction. The payoff of the computational efforts is: long, arduous, and expensive experiments have been modeled and guided using “virtual experiments” on computers, saving time and resources.

CWO

Climate
Weather
Ocean Modeling

CWO focuses on the accurate numerical simulation of the Earth's atmosphere and oceans on those space and time scales important for both scientific understanding and DoD operational use. This CTA includes the simulation and forecast of atmospheric variability (e.g., temperature, winds, pressure, relative humidity, cloud cover, precipitation, storms, aerosols and trace chemicals, surface fluxes, etc.) and oceanic variability (e.g., temperature, salinity, currents, tides, waves, ice motion and concentration, sediment transport, optical clarity, etc.). Numerical simulations and real-time forecasts are performed from the very top of the atmosphere to the very bottom of the ocean. CWO also includes the development of numerical algorithms and techniques for the assimilation of *in situ* and remotely sensed observations into numerical prediction systems. CWO has DoD applications on a daily basis for specific warfare areas, mission planning, and execution (air, ground, sea, and space), as well as for flight and sea safety, search and rescue, optimal aircraft and ship routing, and weapon system design. This CTA provides DoD with (1) real-time, high-resolution weather and oceanographic forecasts leading to incisive decision making and enhanced operational capability in adverse weather and ocean conditions, and (2) realistic simulations of the dynamic oceanic and atmospheric environment to permit effective mission planning, rehearsal and training, and materiel acquisition.

Title: Eddy-Resolving Global and Basin-Scale Ocean Modeling
Author(s): A.J. Wallcraft, E.J. Metzger, P.G. Posey, and J.F. Shriver
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

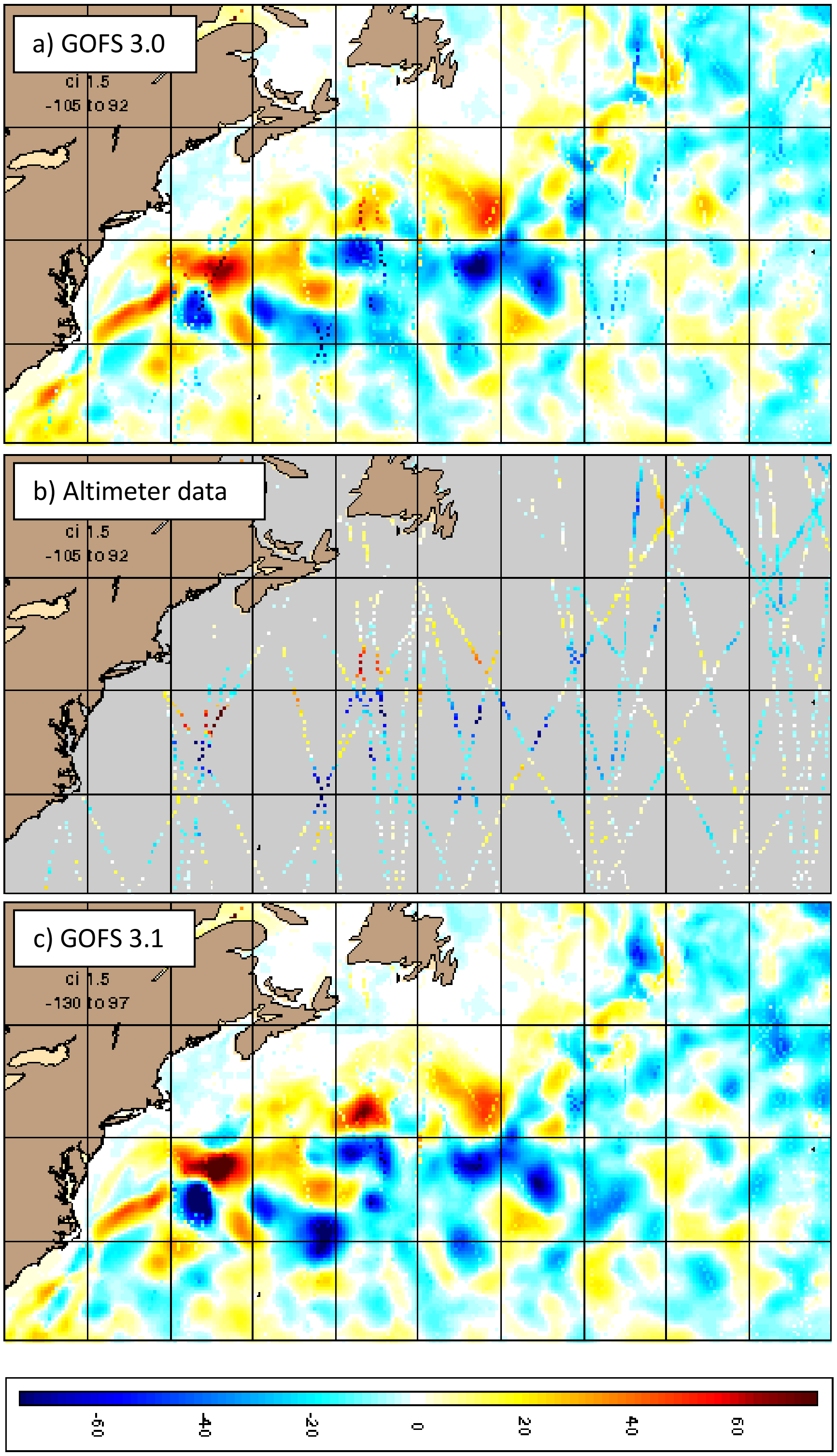
Computer Resources: IBM iDataPlex, Cray XC30, Cray XC40 [NAVY, MS]; Cray XE6 [ERDC, MS]

Research Objectives: Modeling component of a coordinated 6.1-6.4 effort on the "Grand Challenge" problem of eddy-resolving global and basin-scale ocean modeling and prediction. This includes increased understanding of ocean dynamics, model development, model validation, naval applications, oceanic data assimilation, ocean predictability studies, observing system simulation studies, and nested models.

Methodology: The appropriate choice of the vertical coordinate is a key factor in OGCM design. Traditional ocean models use a single coordinate type to represent the vertical, but no single approach is optimal for the global ocean. Isopycnal (density tracking) layers are best in the deep stratified ocean, Z-levels (constant depths) provide high vertical resolution in the mixed layer, and terrain-following levels are often the best choice in coastal regions. The HYbrid Coordinate Ocean Model (HYCOM) has a completely general vertical coordinate (isopycnal, terrain-following, and Z-level) via the layered continuity equation.

Results: 11 refereed paper articles published in FY16.
Global modeling: The $1/12^{\circ}$ (equatorial) global HYCOM system with Navy Coupled Ocean Data Assimilation (NCODA) has been run daily by NRL since December 2006. This Global Ocean Forecast System (GOFS) 3.0, with a seven-day forecast, was declared operational at NAVOCEANO on 20 March 2013. For real-time and archived results, see http://www7320.nrlssc.navy.mil/GLBhycom1-12/skill.html. Its follow on, GOFS 3.1, will be transitioned from NRL to NAVOCEANO by the end of 2016. It adds the Los Alamos Community Ice CodE (CICE) and several other enhancements. The figure compares the effectiveness of assimilating satellite altimeter observations into GOFS 3.0 and GOFS 3.1. Globally, GOFS 3.0 is capturing 68% of the altimeter signal versus 96% for GOFS 3.1. We are in the process of performing a full year hindcast of GOFS 3.1, forced by NAVGEM 1.4, for the Validation Test Report (VTR), and we are confident that it will perform equal to or better than GOFS 3.0 on a wide range of metrics.
Arctic Modeling: The Arctic Cap Nowcast/Forecast System (ACNFS) consists of HYCOM coupled to the Los Alamos Community Ice CodE (CICE) on the part of our standard $1/12^{\circ}$ global tri-pole grid north of 40_N with NCODA data assimilation of ocean state and sea ice concentration. It has run in real-time since June 2010, and was declared operational at NAVOCEANO in September 2013. For real-time and archived results, see http://www7320.nrlssc.navy.mil/hycomARC/skill_public.html. This year we have started investigating the assimilation of satellite-based sea ice thickness into ACNFS. So far we have only done this for full monthly mean fields as a hindcast, but initial results look promising with the initial improved ice thickness skill being maintained for several months without further assimilation of ice thickness. Earth System Prediction Capability: The Earth System Prediction Capability (ESPC) is a national, multi-agency, collaborative effort to develop the next generation whole earth prediction system. The Navy's ESPC system includes atmosphere, ocean, sea ice, and waves components in fully coupled mode including ensemble prediction. We participated in the 2016 Sea Ice Prediction network (SIPN) Sea Ice Outlook (SIO) using an eleven member time-lagged ESPC ensemble with initial conditions from early May 2016. Results are at https://www.arcus.org/sipn/sea-ice-outlook/2016/june.

DoD Impact/Significance: Data assimilative eddy resolving models are important components of global ocean and sea ice monitoring and prediction systems. Military and civilian applications include ship routing, search and rescue, antisubmarine warfare, coastal and mine warfare, fisheries forecasts, pollutant spill risks, El Niño forecasting, ocean observing system simulation, and global change studies.



The center panel (b) shows sea surface height anomaly (SSHA) (cm) along altimeter tracks that are assimilated into both systems, July 1, 2014, in the Gulf Stream region. The top panel (a) shows the resulting steric SSHA field from GOFS 3.0 with the altimeter track values superimposed, and the lower panel (c) shows the steric SSHA from GOFS 3.1.

Title: Modeling Cloud-Aerosol Interactions in Long-Lived Polluted Clouds
Author(s): P. Caffrey and S. Rabenhorst
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: CWO

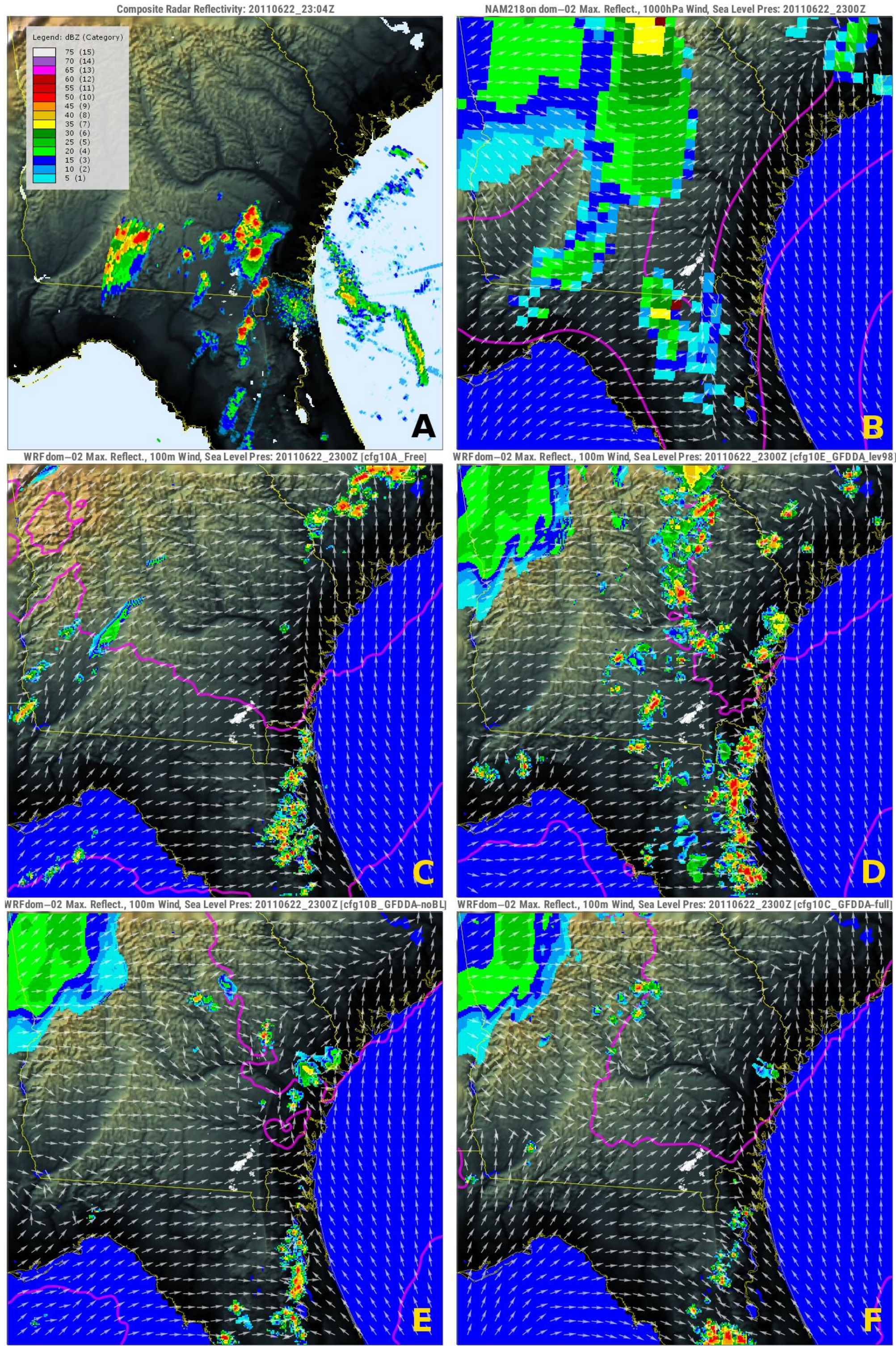
Computer Resources: SGI ICE X [AFRL, OH]; [ERDC, MS]

Research Objectives: We are investigating case studies of heavy aerosol loadings into the upper troposphere/lower stratosphere region through pyro-cumulonimbus and dust-storm events. These strong aerosol loadings are known to produce peculiar signatures in remotely-sensed ice-cloud data, so modeling efforts in this research will further investigate cloud-aerosol interactions, impact (direct, indirect, and semi-direct effects), cloud lifetime, and whether the model is able to correctly reproduce these anomalous events. A combined synergistic model-observation approach is needed to understand fundamental science questions related to cloud-aerosol interactions that will, as time permits, lead to modeling improvements and better forecasting and climate projections.

Methodology: Case study modeling utilizes the chemistry version Weather Research and Forecasting atmospheric model (WRF-Chem) interfaced with a separate fire spread module (SFIRE) to simulate fully coupled wildfire behavior. WRF-Chem's wide ranging model options (physics, numerics, configurations, etc.) are ideal for extensive sensitivity testing, which can be used to elucidate key factors contributing to storm evolution. In most cases the exact mechanisms that trigger specifically a pyrocumulonimbus storm, and the microphysical properties that allowed such longevity, are currently unknown. Therefore, our research leverages the HPC computing environment for multiple high resolution simulations of events to explore model sensitivities to meteorology, land surface interaction, and wildfire contribution for comparison with remotely sensed observations. Model validation is an integral component of this research and will be used to assess how well the model can reproduce these types of phenomenae, and to what extent existing parameterizations can be refined to improve model simulations.

Results: This past fiscal year, two case studies were investigated using the Weather Research and Forecasting model. First, a wildfire case near Fairbanks, Alaska was simulated at kilometer-scale resolutions. WRF's terrain-following vertical coordinate did not perform well (becoming unstable) over Alaska's complex topography at very high resolutions. Therefore we developed an innovative algorithm to modify the topography, which improved model stability while preserving small-scale features that are a source for convective triggering. Several sensitivity runs were improved and an optimal set of parameters was found for the meteorology. Secondly, another case study used WRF to investigate the prestorm environment for the intense wildfires (and subsequent pyroCb) near the Okefenokee National Wildlife Refuge in Georgia. It was found that several factors came together to trigger the storm, including a subtle sea breeze in a conditionally unstable environment. Four dimensional data assimilation was required to improve the pre-storm meteorology. Sensitivity runs once again helped illuminate relevant model parameters for improvement. Findings from the first phase of our project, accurately simulating the meteorology, were necessary for the second phase of our project in which we begin smoke emissions and transport, and comparing pristine verses polluted simulations that explore cloud-aerosol interactions.

DoD Impact/Significance: This modeling work contributes to our understanding of upper troposphere/lower stratosphere aerosol-cloud interactions and lifecycles, which will directly improve DoD's ability to predict cloud and visibility forecasting, and to further improve climate and global aerosol transport modeling.



An example of WRF sensitivity testing. Contours are sea level pressure, vectors are ~100 m wind field, and shading is radar reflectivity. Panels show [A] NEXRAD observations in Jacksonville, Florida, [B] NAM model, [C] WRF “Free-Run” simulation, [D] WRF ~30% increase in vertical levels, [E] WRF using Four Dimensional Data Assimilation (FDDA) above Planetary Boundary Layer (PBL), and [F] WRF with FDDA on all levels. With all other options remaining constant, this demonstrates the difficulty in accurately reproducing the pre-storm environment given the tremendous variability.

Title: Variational Data Assimilation
Author(s): S. Smith,[1] C. Amerault,[2] C. Barron,[1] T. Campbell,[1] S. Carroll,[3] M. Carrier,[1] J. Dastugue,[1] S. deRada,[1] E. Douglass,[1] P. Martin,[1] J. May,[1] H. Ngodock,[1] C.D. Rowley,[1] J.F. Shriver,[1] O. Smedstad,[3] P.L. Spence,[3] and M. Yaremchuk[1]
Affiliation(s): [1]Naval Research Laboratory, Stennis Space Center, MS; [3]Naval Research Laboratory, Monterey, CA; [2]QinetiQ North America, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM iDataPlex, Cray XC30, Cray XC40 [NAVY, MS]

Research Objectives: The scope of this project is to advance the analysis and prediction capability of the Navy's environmental modeling and forecasting systems through the improvement of the assimilation software. Three variational assimilation systems were primarily used in this project: (1) Relo NCOM (3DVAR), (2) the adjointless 4DVAR, and (3) the NCOM-4DVAR. There were seven funded NRL projects that focused on either adding or improving capabilities of 4DVAR in FY16, and the experiments performed under this HPC project went towards satisfying these efforts.

Methodology: The advancement of 4DVAR assimilation systems was supported by the following funded NRL projects in FY16: (1) The 6.4 Ocean Data Assimilation project was tasked to develop separate NCODA preparation software designed solely for the NCOM-4DVAR system and to integrate the NCOM-4DVAR within the operational COAMPS system. (2) The 6.2 Coupled Ocean-Atmosphere Variational Assimilation and Prediction System is coupling the four-dimensional variational (4DVAR) capabilities of the atmospheric and oceanic components of the Coupled Ocean/Atmospheric Mesoscale Prediction System (COAMPS). (3) The 6.2 Coupled Ocean-Acoustic Assimilative Model is coupling the NCOM-4DVAR with the 4DVAR of the acoustic model RAM. (4) The 6.2 Smart Glider Teams for Rapid Update of Local Analysis project is developing and testing a tool for glider team guidance in a dynamic ocean region resolved at tactical scales using NCOM-4DVAR to preserve the fidelity of their collective observations. (5) For the 6.2 Calibration of Ocean Forcing with satellite Flux Estimates project, a whole suite of NCOM-4DVAR experiments were performed for the southern California domain and the North Arabian Sea to examine the impact of heat fluxes on the assimilation system. (6) The 6.1 adjointless 4DVAR for operational Navy ocean models project performed a number of experiments in the Adriatic Sea comparing the performance between the 4DVAR and NCOM-4DVAR systems. (7) The 6.1 Propagation and Dissipation of Internal Tides on Coastal Shelves project is using the NCOM-4DVAR system to assess the accuracy of internal tides and tidal dissipation along the Northwest Australia Shelf.

Results: Numerous NCOM-4DVAR experiments were performed under this FY16 HPC project with the overall result of further improving the analysis accuracy, prediction skill, portability and robustness of the system. Even though the NCOM-4DVAR system has already been transitioned to NAVO, much effort was performed this fiscal year to improve its capabilities. Advancements were also made in: the understanding of the modeling and prediction of internal tides and heat fluxes, the coupling of assimilation systems from different models, and glider control. Finally, results from the adjointless 4DVAR methodology show that it potentially can be a more efficient alternative to NCOM-4DVAR.

DoD Impact/Significance: The 3D and 4D variational systems that were tested under this project went towards improving the Navy’s capability of forecasting the Ocean environment. Various validation studies for the NCOM-4DVAR were performed and showed a more accurate analysis and model forecast fields than its predecessor, Relo NCOM. Additionally, the work on coupling the assimilation systems for the ocean, atmosphere, and acoustic models made significant progress this fiscal year and these coupled systems will ultimately further improve the forecast skill of all three environments.

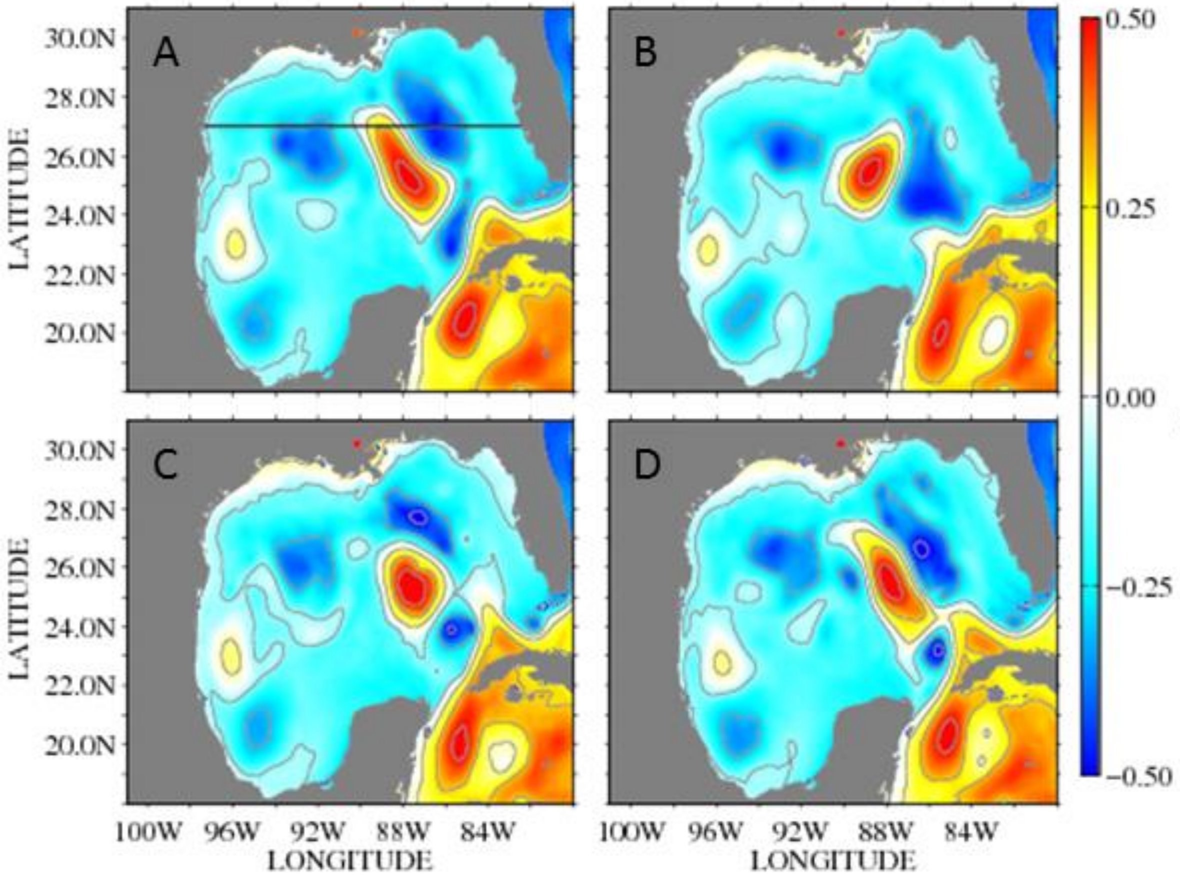


Figure 1. Sea Surface Height maps from a twin data experiment in the Gulf of Mexico showing the impact that the upcoming Surface Water and Ocean Topography (SWOT) satellite altimeter will have on the NCOM-4DVAR Assimilation and Forecasting system. (A) The nature run, which is considered the "truth" of which observations are sampled from. (B) The free run is from just the forecast model with error purposefully added to it. (C and D) NCOM-4DVAR analyses resulting from assimilating simulated SSH observations along conventional altimeter tracks that are (C) currently available and (D) the future SWOT tracks that are anticipated.

Title: Multi-Scale Characterization and Prediction of the Global Atmosphere from the Ground to the Edge of Space Using Next-Generation Navy Modeling Systems

Author(s): J.P. McCormack,[1] S.D. Eckermann,[1] F. Sassi,[1] K.W. Hoppel,[1] D.D. Kuhl,[1] D.R. Allen,[1] J. Ma,[2] C. Metzler,[1] and J. Tate[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]Computational Physics Inc., Springfield, VA
CTA: CWO

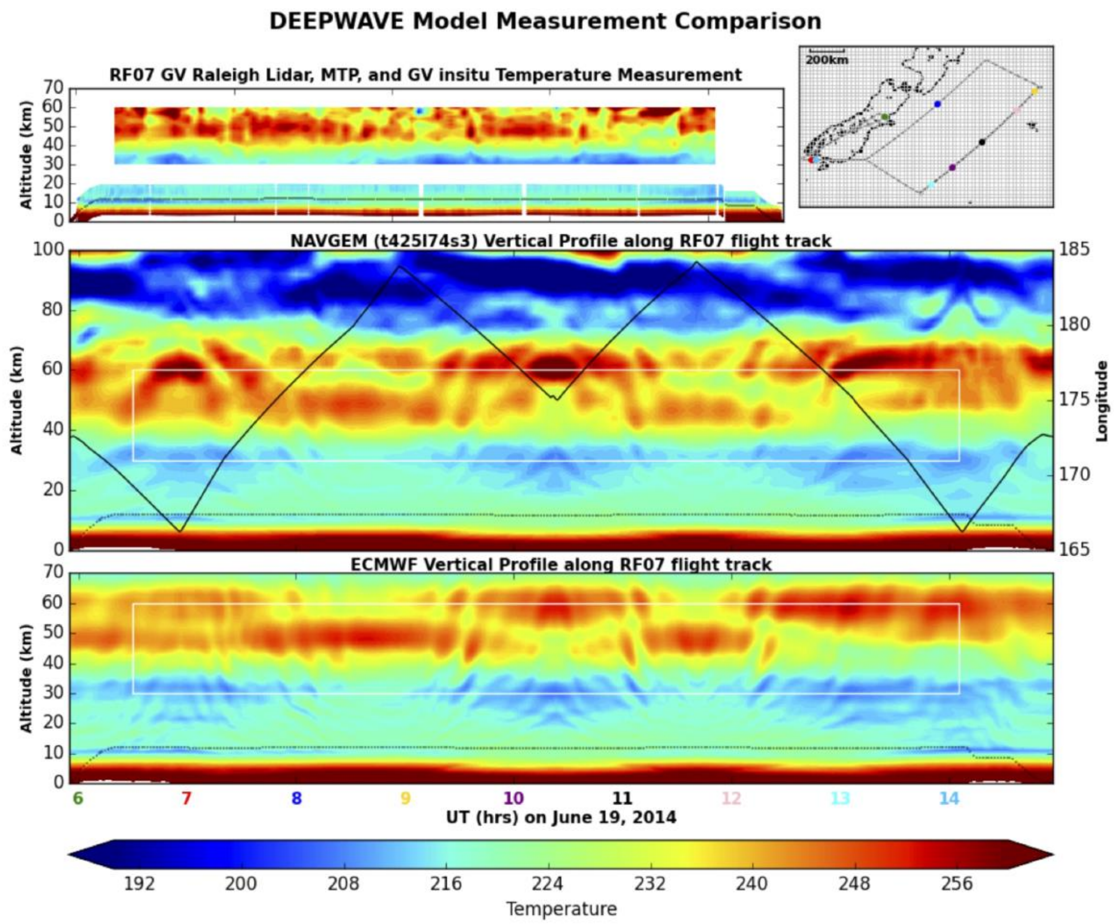
Computer Resources: Cray XC40 [ARL, MD]; [NAVY, MS]; Cray XC30 [AFRL, OH]; [NAVY, MS], IBM iDataplex [NAVY, MS]; [MHPCC, HI]; Cray XE6 [ERDC, MS]; SGI Altix ICE [NRL, DC]

Research Objectives: To develop and test new seamless atmospheric specification and prediction capabilities from 0 to 500 km altitude for a future Navy Earth System Prediction Capability (ESPC) linking the ocean, atmosphere, and space over time scales from hours to decades.

Methodology: This project develops and tests key components of state-of-the-art systems required for the improved modeling, prediction and analysis of the extended operational environment for Navy applications, focusing on the atmosphere, the near space and the geospace. Specific systems under development are: (a) the Navy Global Environmental Model (NAVGEM), the Navy's operational global numerical weather prediction (NWP) system; (b) the NRL Atmospheric Variational Data Assimilation System–Accelerated Representer (NAVDAS-AR), the Navy's four-dimensional variational (4DVAR) data assimilation algorithm; (c) the Coupled Ocean-Atmosphere Mesoscale Prediction System (COAMPS®), the Navy's operational regional NWP system, and; (d) the Whole Atmosphere Community Climate Model Extended Version (WACCM-X), a ground-to-space global model of Earth system climate and part of the National Center for Atmospheric Research Community Earth System Model (NCAR CESM).

Results: Major results directly facilitated by HPC resources during FY16 include (a) development and testing of a new, highly scalable ensemble-based 4DVAR assimilation algorithm in NAVDAS-AR; (b) improved NAVGEM model physics at high altitudes that removes a persistent cold bias in stratospheric and mesospheric temperature forecasts; (c) development of a stratospheric ozone assimilation capability as a new source of information on high-altitude winds and temperatures; (d) validation of diurnal and semidiurnal tides in NAVGEM mesospheric wind analyses through comparison with independent ground-based observations; (e) production runs of high horizontal resolution NAVGEM meteorological analyses extending from the surface to 100 km altitude during the Deep Propagating Gravity Wave Experiment (DEEPWAVE) field campaign of June-July 2014 as part of a comprehensive study of atmospheric dynamics, which also included aircraft-based observations and analyses from the European Centre for Medium Range Weather Forecasting (ECMWF); (f) development of high-altitude NAVGEM analyses as initial conditions for extended COAMPS® simulations; and (g) first use of high-altitude NAVGEM analyses for specification of lower atmosphere dynamics in WACCM-X model simulations of the 2009–2010 Northern Hemisphere winter.

DoD Impact/Significance: This research directly addresses Navy requirements to develop and test new high-altitude atmospheric specification and prediction capabilities that together will comprise bridge technology to a future Navy ESPC by 2020. The direct benefit this project provides to the Navy is logistical support to install an accurate high altitude (e.g., 10–100 km altitude) specification and forecast capability in the NAVGEM and COAMPS systems, which can ultimately provide improved near-space specification and prediction capabilities to the warfighter over both tactical and strategic time frames.



Top right-hand corner: Flight track of Gulfstream V aircraft on DEEPWAVE flight of 19 June 2014. *Top left-hand corner*: Altitude-time section of observed temperatures from onboard instruments. *Middle*: Altitude-time section of high-altitude NAVGEM temperature analyses along the flight track; black line indicates flight track longitude. *Bottom*: Corresponding temperatures from ECM WF analyses.

Title: Advanced Coastal Ocean Modeling

Author(s): C.A. Blain[1] and M.K. Cambazoglu[2]
Affiliation(s): [1]Naval Research Laboratory, Stennis Space Center, MS; [2]University of Southern Mississippi, Dept. of Marine Science, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM iDataPlex [NAVY, MS]

Research Objectives: The objectives are to develop and evaluate the capabilities of a finite element-based coastal ocean model applied to riverine environments. The high performance computing work undertaken in FY16 has focused on application of the Advanced Circulation Model, ADCIRC, to study river-floodplain interactions within Lower Pearl River Basin (LPRB), a braided river system.

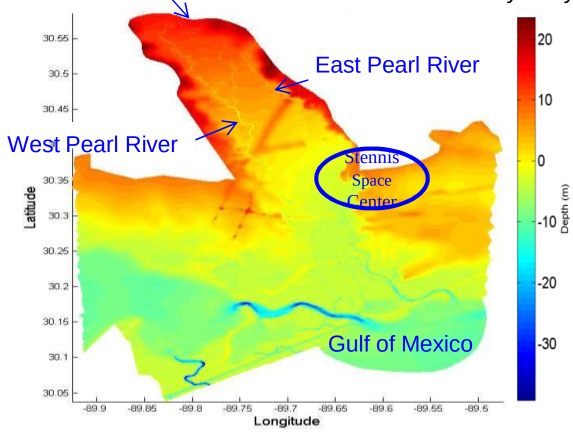
Methodology: Construction of a hydrodynamic modeling system for the Lower Pearl River Basin was completed during FY16. A channelized mesh of the East and West Pearl Rivers, including its complex braided channels, was joined to the surrounding floodplain. The floodplain covers areas between the channels as well as those regions outside the channels that form the catchment basin. The entire domain extends from a boundary located downstream of Bogalusa, LA at which river discharge is specified to a boundary just beyond the Mississippi Sound in the open waters of the Gulf of Mexico at which water level forcing (tides and surge) is applied. Spatial resolution ranges from 3 m to 1.4 km, with the highest resolution reserved for river channels; the mesh itself contains 422K nodes and 843K elements. Sensitivity analyses to assess the river-floodplain interaction have been conducted via 14-day simulations considering upstream discharge at high, average and low flow conditions, varying spatial distributions of Manning's friction coefficient, initial river elevation, and channel depths. Challenges include treatment of overbank flow and full bank conditions for those portions of the basin that lie above mean sea level.

Results: The first high resolution hydrodynamic model of the LPBR and it floodplain is created and successfully simulates river-floodplain interaction at low, average and high flow conditions according to discharge records available at the NOAA Bogalousa, LA, station. A novel semi-automated approach to the integration of the channel model with the floodplain was employed using the NRL patented NUMCAT tools. Achievement of this groundbreaking work led to ADCIRC model developments that stabilize high resolution, implicit solutions of the diagonally dominant, GWCE continuity equation. An offset to the bathymetric depth is required to eliminate negative values on the diagonal of the GWCE solution matrix. The negativity arises when there are large numbers of nodes (high resolution) above mean sea level (negative depths). The validation test case for the LPRB is H. Isaac, 2012, both a surge and rainfall threat. NOAA's best available reanalysis h*Wind product was processed and applied to the Louisiana Coastal Protection and Restoration Authority surge and inundation mesh. LPRB offshore water level forcing is extracted from this large domain simulation of H. Isaac. Upstream hydrographs are processed from NOAA discharge station data at Bogalousa, LA. Validation hydrographs provided by NOAA NWS LMRFC guide adjustments to river depths throughout the braided river system, which contain a great deal of uncertainty. A transition plan has been developed for the LPRB model with transition partners: St. Tammany Parish, LA, NOAA NWS-Lower Mississippi River Forecast Center, and the targeted operational venue at the LSU Center for Coastal Resiliency, Coastal Emergency Risk Assessment office.

DoD Impact/Significance: An operational strategy of applying high resolution finite element coastal models to challenging river-floodplain environments results in the fine scale prediction of rivers, tides, currents and water elevation that impact coastal missions related to Special Warfare, Mine Warfare and amphibious operations. The technology developed is capable of water level predictions under extreme surge, tide and rainfall conditions.

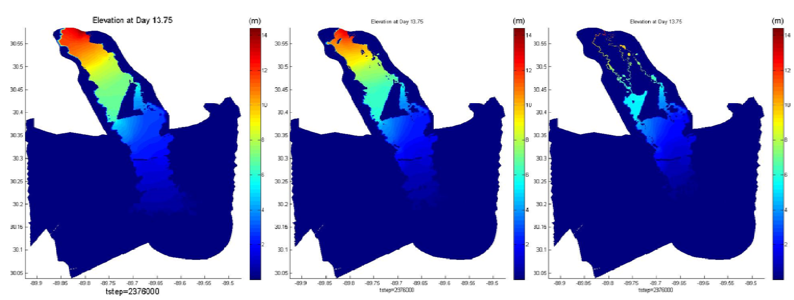
River-Floodplain Interactions
On the Lower Pearl River Basin, LA/MS

A)



A) The first ever, realistic model of the Lower Pearl River Basin, LA/MS, using the ADCIRC coastal model.

B) C) D)



Computed water levels in the Lower Pearl River Basin at B) high flow (40,000 cfs), C) average flow (10,000 cfs), and D) low flow (3000 cfs) conditions.

Title: Coastal Mesoscale Modeling—COAMPS-TC
Author(s): P.A. Reinecke
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: Cray XE6 [ERDC, MS]

Research Objectives: Accurate tropical cyclone (TC) prediction is one of the great challenges for the meteorological forecasting community. While steady advances in global numerical weather prediction (NWP) have led to a significant improvement of TC position guidance, similar gains have not been achieved for intensity forecasting. Fundamental predictability limitations of mesoscale convective motions within TCs motivate the need for a probabilistic prediction system capable of quantifying these uncertainties. Over the last several years, the Office of Naval Research (ONR) and PMW-120 sponsored NRL to develop COAMPS-TC, a new state-of-the-science NWP system designed specifically for the simulation of tropical cyclones in support of Navy and DoD operations, as well as for civilian applications. As part of this effort, researchers at NRL developed and tested a probabilistic prediction system, based on an initial condition ensemble, designed to quantify the inherent uncertainty associated with TC forecasting. The objectives of this HPC project are two-fold: first, test and validate the system for a large sample of TC cases in order to verify statistically meaningful results; second, generate real-time probabilistic TC forecasts over the Atlantic and Pacific Ocean basins. This second objective is part of a larger community effort, funded by the Hurricane Forecast Improvement Project (HFIP), to provide probabilistic predictions based on a suite of different dynamical TC models in order to better characterize the uncertainty associated with TC prediction.

Methodology: The stochastic nature of the atmosphere requires that changes to the NWP system be fully tested over a large sample of cases to obtain statistically significant results. To this end, a sample of approximately 300 historical storms was selected for retrospective verification. A 10-member COAMPS-TC ensemble was constructed using climatological initial-condition perturbations centered on a deterministic analysis. The 10-member ensemble was simulated to a 120-h lead time and evaluated against position and intensity observations. Every incremental change to the system, such as the decrease of the horizontal resolution from 5 to 3 km, or a change to the physical parameterizations must undergo similar testing procedure in-order to evaluate the impact of the change. Second, the system was run in real-time in-order to evaluate its performance in an environment similar to the operational conditions at FNMOC. The 10 member COAMPS-TC ensemble was combined with a 20-member HWRF ensemble and the probabilistic track and intensity forecasts are disseminated via a publicly available web page.

Results: For FY16 several configurations of the ensemble COAMPS-TC system were rigorously tested over a suite of storms in the Atlantic and Pacific Ocean basins from the 2014. Variations on the methodology to perturb the initial model conditions were tested. The system was run in real-time for both Atlantic and Pacific Ocean basins for the end of the 2015 season and the beginning of the 2016 season. Several new probabilistic TC products were developed for the real-time system. Figure 1 shows one such product, which concisely displays the ensemble position and intensity spread for Hurricane Joaquin and Hurricane Patricia, the strongest Hurricane ever recorded in the Western Hemisphere. Hurricane Joaquin was responsible for sinking the SS El Faro near the Bahamas.

DoD Impact/Significance: Tropical cyclones are a significant forecasting challenge for Fleet operations. Using ensemble prediction to quantifying the inherent uncertainty associated with TC position and intensity forecasts with ensemble prediction will result in enhanced Fleet safety and reduced Navy costs. The HPC DSRC provides a unique environment to test and improve the COAMPS-TC probabilistic forecast system prior to transition for operation use at FNMOC. These improvements will inform future decisions regarding the design of probabilistic TC prediction systems.

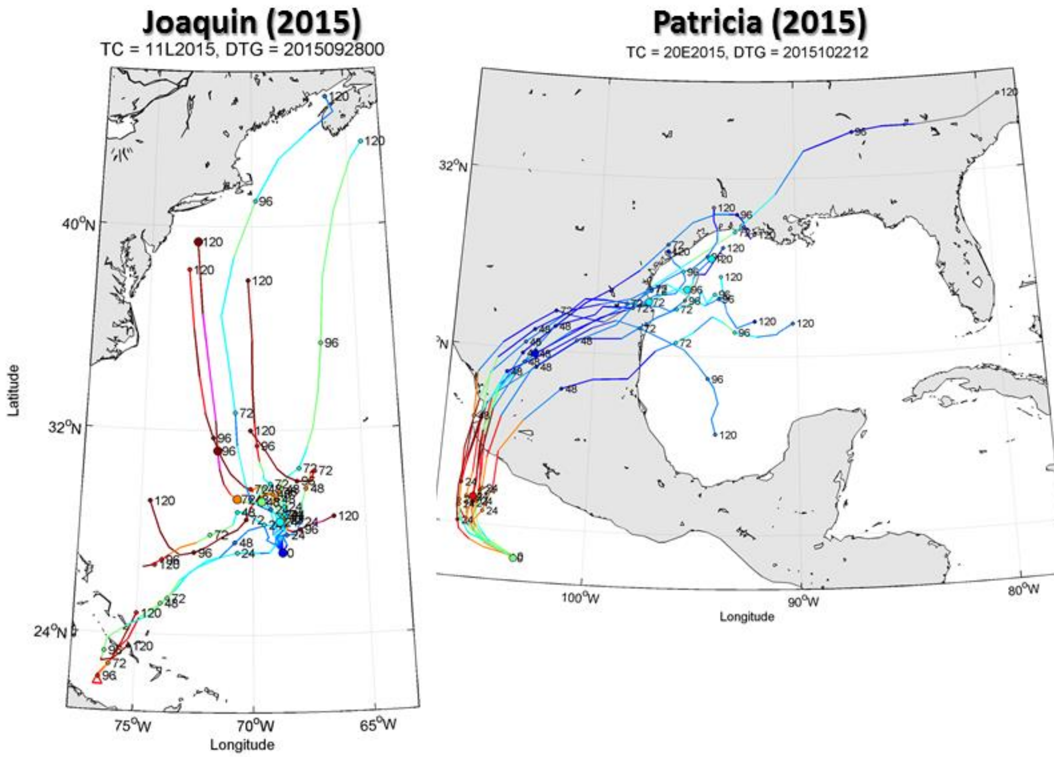


Figure 1. Ensemble position and intensity forecast for a single forecast of Hurricane Joaquin (2015) and Hurricane Patricia (2015). Hurricane Joaquin was responsible for the sinking of the SS El Faro, a container ship. Hurricane Patricia was the strongest storm ever recorded in the Western Hemisphere.

Title: Dynamics of Coupled Models
Author(s): I. Shulman, P.J. Sakalaukus, B. Penta, and S. Cayula
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM iDataPlex [NAVY, MS]

Research Objective: Improve our understanding of coupled bio-optical and physical processes in the coastal zone and the variability and predictability of the coastal ocean's optical properties on time scales of 1–5 days. Investigate the coupled dynamics of ocean bio-optical, physical and atmospheric models. Provide a foundation for the development of scientifically valid, dynamically coupled atmosphere-ocean models.

Methodology: The approach is based on using nested, coupled physical-bio-optical models of the coastal region together with bio-optical and physical in-situ and remotely sensed observations. Data assimilation techniques for both physical and bio-optical fields are being used to examine project research issues and objectives. The approach is also based on joint studies of the bioluminescence (BL) potential and inherent optical properties (IOPs) over relevant time and space scales. Dynamical, biochemical, physical and BL potential models are combined into a methodology for estimating BL potential and night-time water-leaving radiance (BLw).

Results: We set up numerical models (including BL potential model) for the Delaware Bay area, where observational programs are being conducted. The BL model is based on BL predictions with an advection-diffusion-reaction model (ADR), with velocities and diffusivities taken from the 0.5 km circulation model of the Delaware Bay. The BL model consists of dynamical initialization of the ADR model by assimilating available BL observations, and forecasting BL potential with the ADR model. We conducted preliminary modeling of BL potential and produced the nighttime water-leaving radiance (BLw) and diver/platform vulnerability maps/movies for Delaware Bay area. We investigated the development of the submesoscale filament with elevated chlorophyll-a and BL potential values in the area of interaction of lighter water masses of the Delaware Bay outflow with denser upwelled water. We demonstrated that ageostrophic secondary circulation (ASC) cells contributed to the development of the filament.

We investigated the impact of the errors in the surface photosynthetically available radiation (PAR) values and in the vertical attenuation of PAR on the oceanic model heat content. We demonstrated that with the decrease in water clarity, the relative error in surface PAR introduces a larger error in the model heat content than the same magnitude relative error in the attenuation coefficient. We studied how the model heat budget sensitivities to errors in PAR and its attenuation change in space and time. Derived sensitivities provide a capability to understand and control the impact of errors in PAR and its attenuation on the oceanic model heat budget predictions.

DoD Impact/Significance: Emerging Navy Electro-Optical (EO) systems under development and Special Operations missions require an improved understanding of the ocean optical environment. This is critical for operations and weapon deployment, especially in the coastal and littoral zones. Improved basin scale to mesoscale forecast skill is critical to both military and civilian use of the oceans, particularly on the continental margins.

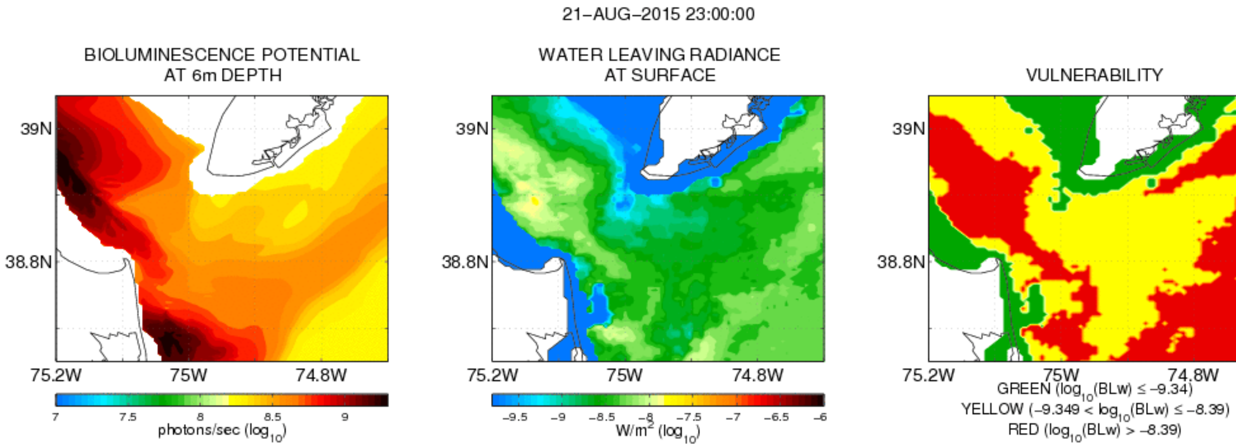


Figure 1. *Left-hand panel:* Forecast of BL potential at 6m depth at the entrance to the Delaware Bay. *Middle panel:* Forecast of water-leaving radiance at surface if we stimulate BL potential at 6m depth. *Right-hand panel:* Forecast of Vulnerability Risk if we stimulate BL potential at 6m depth (based on the minimum intensity of light that could be detected by a dark-adapted eye).

Title: Data Assimilation Studies Project
Author(s): W. F. Campbell and B. Ruston
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: IBM iDataPlex, Cray XC30, Cray XC40 [NAVY, MS]; Cray XE6, SGI ICE X [ERDC, MS]; Cray XC30 [AFRL, OH]; IBM iDataplex [MHPCC, HI]

Research Objectives: Data assimilation corrects model analyses of the atmosphere, ocean or surface using non-homogenous observations. This project develops, tests, and improves (1) our 4DVAR assimilation system, which is coupled to the atmospheric global model NAVGEM (Navy Global Environmental Model); (2) fully ensemble-based data assimilation; (3) hybrid ensemble/4DVAR data assimilation; (4) 4DVAR data assimilation for (COAMPS®[1]); and (5) preparation for and test assimilation of new data types. Our goal is to assimilate traditional data (generally *in situ*, e.g., weather balloons, ship or buoy reports) as well as data from a variety of new sources (often space-borne) efficiently and effectively, to provide the best atmospheric analysis, and ultimately improve numerical weather forecast performance. HPC resources are a critical test for assimilation studies to move to next generation fully coupled atmosphere/land/ocean/sea-ice systems.

Methodology: A variety of experimental setups are used to develop and test our global and regional models and data assimilation systems, as well as large datasets of in-situ and satellite-based observations for several summer and winter months.

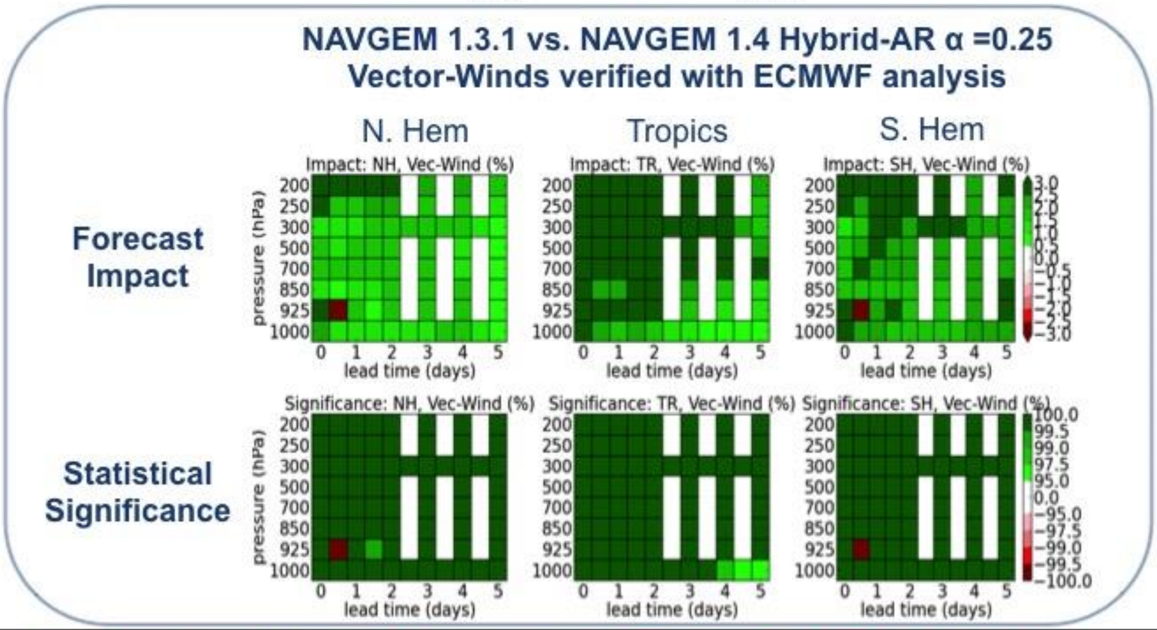
Results: A broad spectrum of research takes place under this project, using both the Navy's latest global (NAVGEM 1.4) and mesoscale (COAMPS) models, and global (NAVDAS-AR and hybrid NAVDAS-AR) and mesoscale (COAMPS-AR) 4DVAR data assimilation systems. Results from FY16 research include the following: (1) computationally intensive pre-operational testing for hybrid 4DVAR; (2) preparation for the assimilation of three new microwave radiance sensors (GMI, AMSR2, and SAPHIR); (3) pre-operational testing of correlated observation error for the ATMS, IASI, and CrIS sensors; (4) the 4-Dimensional COAMPS-AR system has been tested with NAVGEM hybrid 4DVAR boundary conditions and AMSU-A radiance assimilation; (5) an advanced, multiscale ensemble radar data assimilation system has shown notable impact at both the mesoscale and convective scale; and (6) atmosphere-ocean coupled data assimilation has begun testing and shows promise.

DoD Impact/Significance: HPCMP computing platforms provide a common environment for collaboration and the rapid development of NRL's data assimilation systems. The advancements of NAVDAS-AR, NAVGEM (including hybrid NAVGEM), and COAMPS-AR systems have been accelerated by the HPCMP systems. The core and future of Navy data assimilation capabilities are being mostly, and in many cases solely, developed using the resources provided by HPCMP. In summary, the ability to access the HPCMP resources is critical to prepare technology for successful transfer to operations.

[1] COAMPS® is a registered trademark of the Naval Research Laboratory.

Fall/Winter 2014: Oct. 10, 2014-Jan. 7, 2015
90-day Benchmark Testing: NAVGEM 1.4 hybrid DA system
Comparison between NAVDAS-AR 1.3.1 and NAVGEM 1.4 (α =0.25)

$$\mathbf{P}^{\mathbf{f}} = \alpha \mathbf{P}^{\mathbf{f}}_{ENS} + (1-\alpha)\mathbf{P}^{\mathbf{f}}_{CONV}$$



Green Shading → NAVGEM 1.4 is better; Red Shading → NAVGEM 1.3.1 is better

Title: Coastal Mesoscale Modeling
Author(s): P.A. Reinecke
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: Cray XC30, Cray XC40, IBM iDataPlex [NAVY, MS]; Cray XE6 [ERDC, MS]; SGI ICE X [AFRL, OH]

Research Objectives: Our objective is to develop and validate a fully coupled coastal/littoral prediction system that can be used to provide high-resolution (<5 km) data assimilation (DA) and short-term (0-48 h) forecast guidance for tactical sized areas of the world. This system can also be used for basic and applied research leading to an improvement in our understanding of atmospheric and oceanic processes. Improvements to the mesoscale prediction and DA systems will result from this research.

Methodology: The Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMPS®[1]) is being developed further for independent and coupled simulations of the atmosphere and ocean for the mesoscale. The atmospheric component of COAMPS is made up of a DA system; an initialization procedure; and a multi-nested, nonhydrostatic numerical model. This model includes parameterizations for moist processes, surface and boundary-layer effects, and radiation processes. The NRL Coastal Ocean Model (NCOM) is currently being used for the simulation of the mesoscale ocean circulation response to the COAMPS forcing in one-way and two-way interactive modes. Ocean coupling is being developed using the Earth System Modeling Framework (ESMF). A new tropical cyclone capability has been developed for COAMPS, referred to as COAMPS-TC. Development and testing of the Navy's next generation prediction system, NEPTUNE (Navy's Environmental Prediction System Using the NUMA corE) is under way. This system uses a spectral element based approximation to the atmosphere and can scale to over 100,000 cores.

Results: In FY16, COAMPS was demonstrated to be an accurate DA and forecast system capable of predictions and simulations on a variety of horizontal scales of less than 1 km for land-sea effects, topographically driven flows, and tropical cyclones. The COAMPS-TC deterministic and ensemble systems were used for real-time operational planning of the ONR sponsored Tropical Cyclone Intensity (TCI) project. Furthermore, NRL scientists performed extensive validation of the Air-Ocean-Wave coupling in COAMPS for the prediction of the Madden Julian Oscillation (MJO) over the Indian Ocean. In addition to COAMPS progress, significant development of NEPTUNE occurred during 2016, including the inclusion of the GFS physical parametrization packages. Figure 1 shows the 24 accumulated precipitation from a 120-h NEPTUNE forecast, initialized 00 UTC 01 August 2015 using the GFS physics package. Work continues on the development of NEPTUNE with the goal of producing code that can efficiently run on next-generation architectures such as the Intel Knights Landing processors.

DoD Impact/Significance: COAMPS continues to play a significant role in providing atmospheric forecasts in support of Navy missions involving the deployment of weapons systems, strike warfare, radar propagation, and search and rescue. Research and development performed at HPC DSRCs have led to significant improvements in the predictive skill of COAMPS that will greatly benefit the operational performance of COAMPS. The HPC DSRCs will be the primary computing resources in FY2016 and beyond for the development of the fully coupled COAMPS system including the emerging tropical cyclone and ensemble capabilities for COAMPS as well as NEPTUNE, the next generation global and mesoscale modeling system.

[1] COAMPS® is a registered trademark of the Naval Research Laboratory.

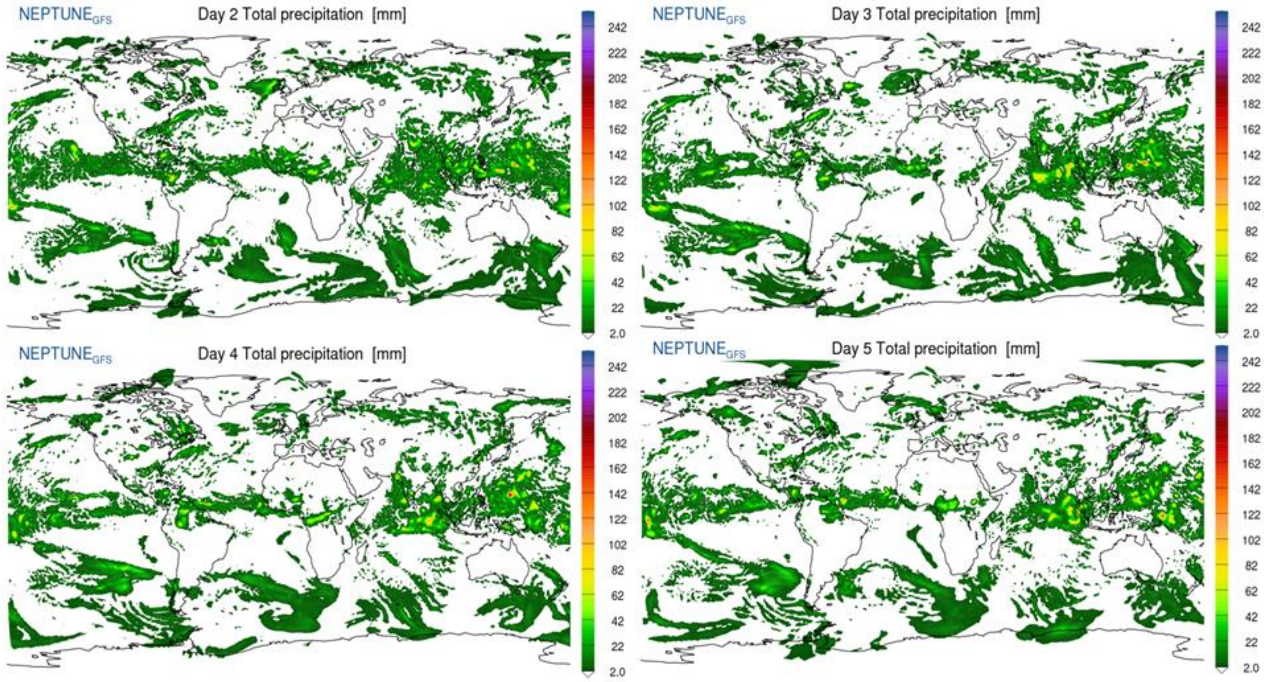


Figure 1. The 24-hour accumulated precipitation (mm) using the GFS physical parameterization package from a 120-h NEPTUNE forecast initialized 00 UTC 01 August 2015. This represents the first spectral element simulation of real-weather data using a full physical parameterization package.

Title: Coupled Ocean-Wave-Air-Ice Prediction System
Author(s): R. Allard, T. Campbell, J. Dykes, D. Hebert, T. Jensen, T. Smith, E. Rogers, and J. Veeramony
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: IBM iDataPlex, Cray XC40 [NAVY, MS]

Research Objectives: Perform validation testing of the Coupled Ocean Atmosphere Mesoscale Prediction System (COAMPS®[1]) which is six-way coupled with the Navy Coastal Ocean Model (NCOM), Simulating Waves Nearshore (SWAN) model and WaveWatch-III (WW3) model via the Earth System Modeling Framework (ESMF). Continue testing the COAMPS-CICE system, which is being developed in 6.2. Utilize the fully coupled system to perform applied research in areas such as the North Arabian Sea and Bay of Bengal by running the model in near real-time.

Methodology: Perform testing of the fully coupled ocean-wave system with data assimilation on the Navy DSRC for four regions run operationally by the Naval Oceanographic Office with a host resolution of 3.7 km and inner nest of 500m. Model hindcast studies will be performed for 9-month periods and evaluated using ocean scorecard metrics. Validation testing for the fully coupled atmosphere-ocean-wave system will be performed for the same four regions and time period (January 1—September 30, 2015). Validation testing will investigate the improvement (if any) of the fully coupled system versus the ocean-wave system.

Results: COAMPS software was ported to the Cray XC40 at the NAVO DSRC during 1QFY16. An evaluation of the ocean-wave system for four operational regions showed that the coupled system performed as well or better than the operational, standalone, NCOM system. Scorecard metrics were used to evaluate temperature and salinity profiles, drifting buoys, and derived parameters such as mixed-layer depth and sonic-layer depth. A regional 2km CICE model was run operationally to support the ONR Sea State fieldwork in the Beaufort/Chukchi Sea for the period of October 1–November 15, 2015. The regional CICE was forced with a 15km COAMPS atmospheric model and used the Global Ocean Forecast System (GOFS 3.1) as ocean input. Ice drift from the regional CICE system was evaluated against ice drift from Cold Region Research Engineering Laboratory Ice Mass Balance Buoys (IMBB) for the period from late summer–early autumn 2016 in the Beaufort Sea (Fig. 1). The model shows good agreement for both ice drift and ice thickness. The regional CICE forecast system was also run to support the Arctic Ice Exercise (ICEX) in March 2016. A regional WW3 domain was run in which CICE inputs (concentration, ice thickness) were used to evaluate new ice source terms in WW3. The fully coupled COAMPS atmosphere-ocean-wave system was run in near real-time to support ONR projects in the Bay of Bengal and North Arabian Sea. The modeling system assimilated real-time ocean observations. NCOM was run with 60 vertical levels; with 20 levels resolving the upper 10m of the water column. The models were coupled every 10 minutes.

DoD Impact/Significance: The development of a coupled air-ocean-wave prediction system can have a pronounced effect on Navy forecasting by improving ASW performance, tropical cyclone prediction, search and rescue and mission planning. The relocatable COAMPS-CICE system will provide high-resolution Arctic forecasting of ice thickness, ice drift and concentration to support navigation.

[1] COAMPS® is a registered trademark of the Naval Research Laboratory.

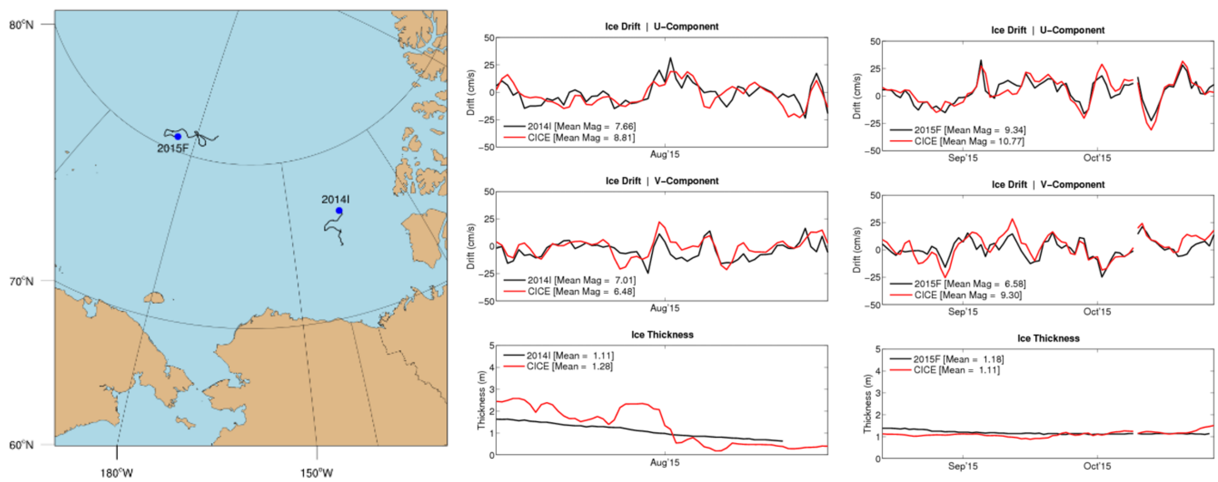


Figure 1. Comparison of the regional CICE model ice drift and ice thickness verses two Cold regions Engineering and Research Laboratory (CRREL) Ice Mass Balance buoys for the period of August–October 2015.

Title: Probabilistic Prediction to Support Ocean Modeling Projects

Author(s): C.D. Rowley,[1] L.F. Smedstad,[1] C.N. Barron,[1] M. Wei,[1] M. Yaremchuk,[1] J. May,[1] J. Dastugue,[1] P.J. Sakalaukus,[1] P.L. Spence,[2] N. VandeVoorde,[2] and B. Maloy[3]
Affiliation(s): [1]Naval Research Laboratory, Stennis Space Center, MS; [2]Vencore, Stennis Space Center, MS; [3]Jacobs Engineering, Stennis Space Center, MS
CTA: CWO

Computer Resources: Cray XC30, Cray XC40, IBM iDataplex [NAVY, MS]

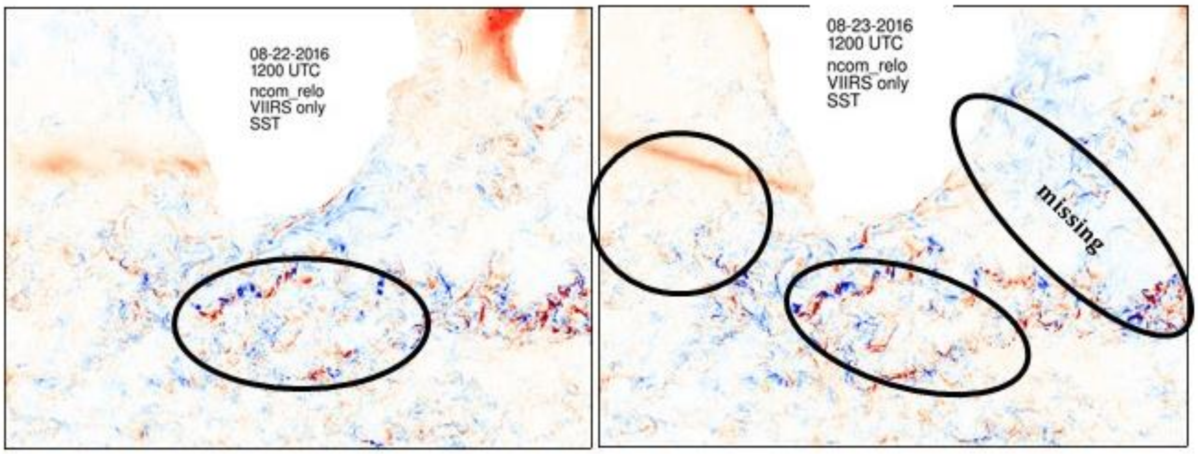
Research Objectives: Develop ocean and air-sea coupled ensemble generation, ensemble data assimilation, and probabilistic prediction capabilities using the Coupled Ocean Atmosphere Mesoscale Prediction System (COAMPS®[1]), Navy Coastal Ocean Model (NCOM), and Hybrid Coordinate Ocean Model (HYCOM). Extend ocean data assimilation capabilities and test and implement new types/platforms of ocean and air/ocean surface observational data.

Methodology: Current operational capability for regional ocean ensemble forecasts is being extended to global ocean and regional and global coupled air-ocean-ice-wave extended-range forecast systems. We face new technical challenges due to the size and scale of global ocean and global coupled ensembles in the Earth System Prediction Capability (ESPC) program. Work consisted of global coupled system ensemble initialization and metrics development; support for NRL modeling and data handling; archive data processing for Fleet Synthetic Training; testing of systems for operational use with new types of input data; NCOM/NCODA system development to support NAVOCEANO operational modeling; assimilation tests comparing adjoint-free and standard 4dVar; and a series of assimilation runs with an NCODA-driven CICE model to compare the standard NCODA formulation of the ice concentration correlation functions with those formulated implicitly in terms of the exponential of the diffusion operator. Sea surface temperature analyses were performed to assess the impact of new data sources at the air-sea interface.

Results: Results of FY16 include progress on global ensemble initialization and metrics implementation, assessment of new sources of observational data for assimilation, and support for transitioned systems. In development of the global ocean ensembles for ESPC, an extended set of ensemble metrics were implemented. In support for Fleet Synthetic Training, a large dataset of a 20-year reanalysis integration of HYCOM was post processed to provide operational data to the fleet. We continue to support transitioned operational NCOM/NCODA systems at NAVOCEANO using the allocation in this project. We tested and transitioned updated code on the NAVY DSRC Cray systems prior to the switch to the new Cray operational system. The adjoint-free 4dVar technique required 10–15 times less wall time as compared to 4dVar, primarily because of its better parallelization capability while delivering comparable forecast skill. The new NCODA correlation function tested in the ice analysis demonstrates 2–6 times faster analysis time with somewhat smoother increments and very similar forecast skill. The sea surface forecasts were used to diagnose combinations of factors for predicting significant dirunal warming events.

DoD Impact/Significance: Higher resolutions and larger ensembles are needed to ensure forecast reliability and accurate risk assessment in areas such as antisubmarine warfare, nuclear-chem-bio hazard prediction and monitoring, and search and rescue. Development of extended-range coupled forecasts depends on probabilistic forecasting, due to the inherent limitations of deterministic forecasts at extended forecast times, and on new coupled-assimilation techniques to improve initial conditions. These HPC resources support research and development efforts on coupled data assimilation and ensemble forecasting. Operational systems are becoming more embedded with new types in data obtained from autonomous systems, and more interest on the air-sea interface requires more understanding of the assimilation capabilities that will improve modeling in these areas. As modeling improves, more information can be shared, with a focus on getting better information to the fleet both in real time operations and in training.

[1] COAMPS® is a registered trademark of the Naval Research Laboratory.



A calculation of sea surface temperature difference between midnight and noon shows three obvious areas of diurnal warming off southern Africa. This is caused by a presence of low wind stress and high solar flux. When only low wind stress is present the diurnal warming does not appear as noted in the oval in the right panel.

Title: Coastal Mesoscale Modeling—COAMPS-TC Intensity Prediction
Author(s): J.D. Doyle
Affiliation(s): Naval Research Laboratory, Monterey, CA
CTA: CWO

Computer Resources: Cray XC30, Cray XC40 [NAVY, MS]

Research Objectives: Tropical cyclone (TC) track forecasts have improved in a steady manner over the past several decades, but intensity forecasting has shown little increase in skill over the same time period. This is due, in part, to our limited ability to properly model physical process controlling tropical cyclone structure and intensity, but also to the inherent sensitivity that tropical cyclone forecasts exhibit to initial conditions. The objective of this project is to further develop and demonstrate COAMPS-TC, a new state-of-the-science numerical weather prediction (NWP) system designed specifically for the simulation of tropical cyclones in support of Navy and DoD operations, and for civilian applications as well. The COAMPS-TC system has been operational at Fleet Numerical Meteorology and Oceanography Center (FNMOC) since June 2013. The overall goal is to improve tropical cyclone intensity predictions using COAMPS-TC through improved vortex initialization and representation of physical processes.

Methodology: There are two types of COAMPS-TC simulations and forecasts that require high-priority computational resources. The first type of application is used to facilitate rapid development and testing of COAMPS-TC. The prototype testing for COAMPS-TC needs to be rigorous and involves running approximately 500 or more individual cases in order to assess the performance of the system in a statistically meaningful manner. Each incremental change in the development process needs to be tested through this procedure. This rapid testing process is needed to develop and evaluate the new version of COAMPS-TC that will be run operationally at FNMOC. A second type of COAMPS-TC application involves the real-time execution of a more advanced experimental version of COAMPS-TC, which contains more advanced capabilities than the FNMOC version, on the DSRC. The testing of the experimental COAMPS-TC system is performed for all tropical cyclones worldwide.

Results: Several configurations of COAMPS-TC were rigorously tested over a suite of storms in the Atlantic and Pacific Ocean basins based on several previous TC seasons. A new version with significant improvements was transitioned to operations at FNMOC in May 2016. These improvements included a fully coupled air-ocean capability (COAMPS-TC nonhydrostatic atmosphere and NCOM), along with upgrades to the physical parameterizations. Figure 1 shows an example of a real-time COAMPS-TC 5-day forecast track and intensity for Super Typhoon Meranti initialized at 1800 UTC September 10, 2016. Typhoon Meranti was one of the most intense tropical cyclones on record, impacting the Philippines, Taiwan, as well China in September 2016. The model forecast track (red) is quite close to the observed best track (black) (Fig. 1). The intensity forecast shows that the model (red) was slow to develop the system relative to the intensity estimates (black); however it is encouraging that COAMPS-TC intensifies the storm to a category 5 intensity. Overall, the COAMPS-TC forecasts for Meranti were quite accurate for track and skillfully predicted the potential for rapid intensification. COAMPS-TC continues to be one of the top performing tropical cyclone prediction models in 2016.

DoD Impact/Significance: Tropical cyclones remain the most disruptive and devastating environmental threat that impact U.S. Navy operations. We anticipate that an increase in accuracy of tropical cyclone forecasts will result in significant cost benefit to the Navy through better sortie decisions and avoidance of hazardous winds and seas. Real-time testing and development of the system at HPC DSRCs have led to significant improvements in the data assimilation and predictive skill of COAMPS-TC and more rapid transitions to operations at FNMOC. These improvements will inform future directions of tropical cyclone and mesoscale model and data assimilation development, particularly as computational power increases allowing for higher resolution capabilities.

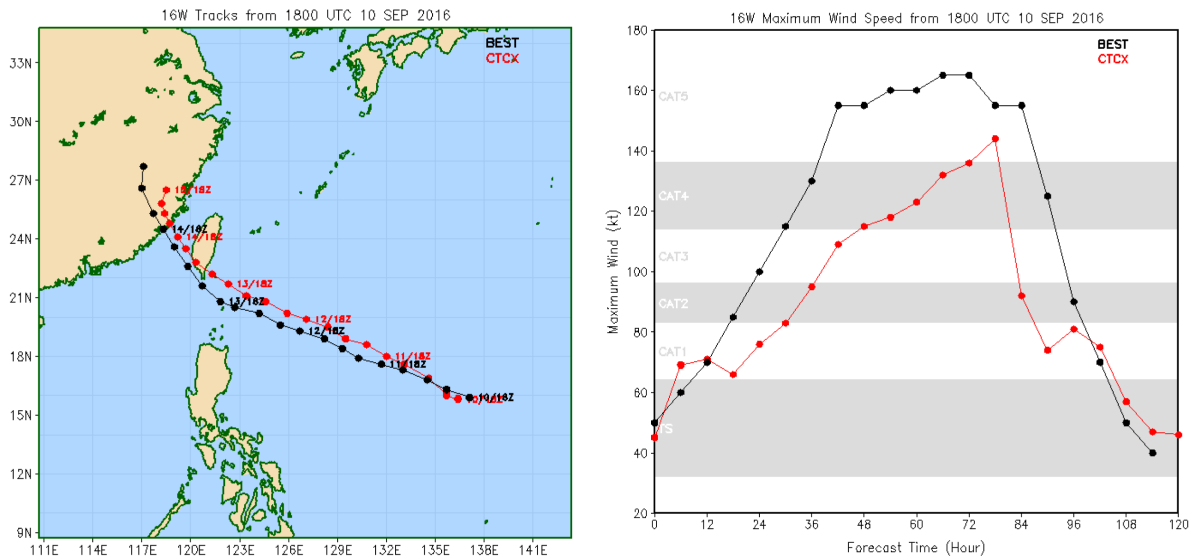


Figure 1. Example of a real-time COAMPS-TC forecast track and intensity for Super Typhoon Meranti, with the forecast initialized at 1800 UTC on September 10, 2016. The observed best track (black) and COAMPS-TC forecast (red) for track (or position) are shown on the left, and for intensity (knots) on the right.

Title: Bio-Optical Modeling and Forecasting
Author(s): J.K. Jolliff, S. Ladner, T. Smith, J. Dykes, and A. Penko
Affiliation(s): Naval Research Laboratory, Stennis Space Center, MS
CTA: CWO

Computer Resources: Cray XC40, IBM iDataplex [NAVY, MS]

Research Objectives: The research objective is to develop and validate three-dimensional, coastal optical prediction systems that leverage results from the Coupled Ocean Atmosphere Mesoscale Prediction System (COAMPS®[1]) and the Navy Coastal Ocean Model (NCOM). The modeling system will forecast the emergence and transport of near shore turbidity plumes and the eruption/propagation of turbidity in the benthic boundary layer. This forecasting capability will be validated and prepared for transition to the Naval Oceanographic Office to be used in support of Navy missions.

Methodology: This project will progress the present optical forecasting capability system forward into a fully three-dimensional context via the following methods: (1) using 3D initialization fields generated via UUV data on the observed relationships between physical and optical gradients; (2) integrating the simulation of bottom boundary layer (BBL) sediment ejection/settling dynamics into the forecasting system; and (3) continually updating the forecast with optical remote sensing data streams. Initial test bed locations for the 3D software system will be placed in areas where NRL observational programs are taking place. The system will require COAMPS and NCOM model output as input to the transport computations. Since these results are on HPC systems, operating in the HPC environment will improve efficiency. As well, the present forecasting system is in serial code; parallelization of the code will improve efficiency and allow for multiple or "ensemble" testing of the pre-operational system.

Results: The Tactical Ocean Data System (TODS) software architecture has been ported to the HPC environment for continuing research and development. The three-dimensional optical generator (3DOG) has been linked to the forecasting software (BioCast) to provide hourly 3D forecasts of the coastal optical environment. The combined system is capable of ingesting satellite data, *in situ* glider/UUV optical data streams, ocean circulation model results, and producing hourly 3D forecasts of the coastal optical environment. An initial test bed was established in the northern Gulf of Mexico, and an additional test bed is being established off the coast of South Korea. Additional model development is being pursued via the linking of bio-optical and seafloor boundary layer models directly into the COAMPS model architecture.

DoD Impact/Significance: The proposed research falls directly within the Naval S&T Strategic Plan Focus Area "Assure Access to the Maritime Battlespace" under the "Match Environmental Predictive Capabilities to Tactical Planning Requirements" objective. U.S. Navy Helicopter Mine Clearance Squadrons (HM-14, HM-15) presently incorporate the helicopter-towed AN/AQS-24 platform into operations. The ability of the AQS-24 platform's laser line scanner (and in the future, streak tube LIDAR, AQS-20) to identify bottom targets is dependent upon the relationships between the tow height and the water column clarity. We anticipate a transition of a fully 3D forecasting system for coastal optics via the Tactical Ocean Data System (TODS) to the Naval Oceanographic Office in FY18. NAVO NP3 and MIW/MCM groups to support mine warfare operations and other missions that are dependent on the performance of Laser/LIDAR systems will use these products.

[1] COAMPS® is a registered trademark of the Naval Research Laboratory.

Title: Atmospheric Process Studies
Author(s): N. Barton,[1] J. Ridout,[1] T. Whitcomb,[1] J. McLay,[1] C. Reynolds,[1] M. Turner[2]
Affiliation(s): [1]Naval Research Laboratory, Monterey CA; [2]Science Applications International Corporation, Monterey, CA
CTA: CWO

Computer Resources: Cray XC30, Cray XC40, IBM iDataPlex [NAVY, MS]; Cray XC40 [ARL, MD]

Research Objectives: The research objectives of this project are to improve our understanding of the fundamental dynamical and physical processes that operate in the atmosphere and to develop and test a state-of-the-art global atmosphere prediction system that includes data assimilation.

Methodology: Our work focuses on improving the accuracy and efficiency of the Navy Global Environmental Model (NAVGEM). NAVGEM is the Navy's current global atmosphere operational numerical weather prediction model, and is used for basic and applied atmospheric research within this project. As initial conditions are very important to numerical system, NAVGEM is developed in conjunction with its data assimilation capability, NAVDAS-AR. In addition, seamless prediction across multiple temporal scales and earth system components is the next frontier of numerical prediction, and NAVGEM is being developed and tested when tightly coupled with the HYbrid Coordinate Ocean Model (HYCOM) and the Las Alamos Community sea ICe Code (CICE) using the Earth System Modeling Framework (ESMF) tools under the Earth System Prediction Capability (ESPC) national program. The focus on seamless prediction across temporal scales requires additional research and development on probabilistic prediction using ensembles.

Results: This year's advances largely fall into three categories: (1) ensemble development, (2) coupled model development, and (3) NAVGEM optimization. Within (1) ensemble development, we are performing basic and applied research. Within basic research, multiple runs of similar forecasts (i.e., ensembles) are being conducted to detect and diagnose the presence of heavy tails in numerical weather prediction. These heavy tails aid in understanding predictability. Within applied research, results include improved ensemble predictions with an updated NAVGEM version (v1.2- T239L50 to v1.3.2- T359L60), updated representation of sea surface temperature variability, and development of extended ranged forecasts from 16 days to 42 days. NAVGEM development associated with the ESPC (2) coupled model focused on improving 30 day forecasts of the Madden Julian Oscillation (MJO). To improve long forecasting of the MJO, enhancements to the convective modified Kain-Fritsch parameterization include a modified cloud top constraint that enhances the ability of the scheme to represent feedbacks between convection and environmental moisture. Preliminary hindcast test results for the DYNAMO period show a significant improvement over the previous default ESPC coupled system physics in the simulated relationship in the tropics between the vertical profile of net moistening and rainfall. Last, (3) NAVGEM optimization focused a new two-dimensional domain decomposition for better scaling across CPUs. With NAVGEM's current one-dimensional domain decomposition significant load imbalances exist at high core counts. With the updated two-dimensional decomposition, NAVGEM is able to run at higher resolutions using larger core counts efficiently.

DoD Impact/Significance: The continued development of our global forecast system is making significant positive impacts on the skill of our weather forecasts and DoD predictions dependent on weather forecasting (i.e., ocean modeling, wave modeling, ship routing). Developments in coupled modeling and extended range-probabilistic forecasting increase the utility of the forecast and potential number of users. This development serves to provide an improved modeling system for studying the dynamical and physical processes in the atmospheric system.

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SIP

Signal Image Processing

SIP covers the extraction of useful information from sensor outputs in real time. DoD applications include surveillance, reconnaissance, intelligence, communications, avionics, smart munitions, and electronic warfare. Sensor types include sonar, radar, visible and infrared images, and signal intelligence (SIGINT) and navigation assets. Typical signal processing functions include detecting, tracking, classifying, and recognizing targets in the midst of noise and jamming. Image processing functions include the generation of high-resolution low-noise imagery and the compression of imagery for communications and storage. The CTA emphasizes research, evaluation, and test of the latest signal processing concepts directed toward these embedded systems. Usually such processors are aboard deployable military systems and hence require hefty packaging, minimum size, weight, and power. System affordability is expected to improve an order of magnitude through the development of scalable codes running on flexible HPC systems. This will enable the traditional expensive military-unique "black boxes" required to implement high-speed signal/image processing to be replaced by commercial-off-the-shelf HPC-based equipment.

Title: Deep Learning Architectures
Author(s): L.N. Smith
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: SIP

Computer Resources: Exxact HD GPU Cluster [NRL, DC]

Research Objectives: In this NRL-sponsored basic research project, we will design, develop, and evaluate novel deep learning algorithms for a variety of applications, such as automated scene understanding, sonar classification, and feature-based tracking. Our motivation is that deep learning is being widely applied commercially but has yet to be tailored for applications of interest to the Navy. Deep learning algorithms can learn directly from data and reason about decision making, hence is a valuable tool for a range of applications. However, there are many open research problems in deep learning that must be solved, such as limited training data, handling noisy data, and combining data from multiple modalities.

Methodology: Our primary methodology is to experiment with many variations of the neural network architecture to determine those modifications that are beneficial, when they are beneficial, and develop an intuition as to why they work.

Results: Scientific: Current research in deep neural networks has already discovered several substantial innovations leading to a continuous stream of scientific publications in high impact journals and conferences. Navy/DoD: New developments in deep learning will assist Navy to apply this technology in a variety of applications. A list of applications include autonomous surveillance; autonomous control of distributed radar systems in a dynamic EM environment; cognitive radar; automatic target recognition; intelligent decision aids, counter UAV systems, and autonomous control of robots and UxVs; cyber security, monitoring, and defense; control of the electromagnetic spectrum; cognitive radios; sonar echo object detection/recognition; situation awareness and target/threat identification and tracking; control of long duration, unmanned underwater vehicles; and Tactical Autonomic Network Control.

DoD Impact/Significance: This research will play a substantial role in the following Navy and DoD future needs:

- Security and force protection in high activity and minimally manned environments (e.g., on littoral combat ship (LCS)).
- Science and technology for efficient, effective cyber capabilities across the spectrum of joint operations.
- New concepts and technology to protect systems and extend capabilities across the electro magnetic spectrum.
- Science and applications to reduce the cycle time and manpower requirements for analysis and use of large data sets.
- Science and technology to achieve autonomous systems that reliably and safely accomplish complex tasks, in all environments.

In addition, advances in deep learning research constantly improve the state-of-the-art results in a host of new applications and this work will bring this expertise to bear on other Navy applications not listed here

SAS

Space and Astrophysical Science

SAS research and development advances understanding, specification, and prediction of the Earth's atmospheric and space domains to exploit the extended operational environment for military advantage and to minimize environmental impacts on military operations. The SAS CTA embodies the use of mathematics, computational science, and engineering in the analysis, design, identification, modeling, and simulation of the space and near-space environment, and of all objects therein, whether artificial or natural. The SAS CTA encompasses foundational discovery research to study the atmospheres of the Sun and the Earth, including solar activity and its effects on the Earth's atmosphere, ionosphere, and near-Earth space, and the unique physics and properties of celestial sources. SAS employs an extensive array of physical and empirical models and analyses tools to integrate observations and theoretical understanding, for ever-improving DoD enterprises within, and exploitation of, the extended operational environment. The CTA melds the strengths of a broad range of physical sciences—atomic and molecular physics, materials science, plasma physics, applied optics, radiation survivability, electronic warfare, directed energy technology, astronautics and space propulsion, orbital mechanics, space situational awareness, and remote sensing—into a structure that helps the DoD multiply force combat effectiveness.

Title: Radiative Signatures and Dynamical Interactions of AGN Jets
Author(s): M.T. Wolff[1] and J.H. Beall[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]St. John's College, Annapolis, MD
CTA: SAS

Computer Resources: SGI Altix ICE [NRL, DC]

Research Objectives: The scientific goal of this research is to investigate the physical processes that occur as an astrophysical jet interacts with the ambient medium through which it propagates. This interaction accelerates the ambient medium, and heats and entrains that material, producing radiation signatures that can be modeled with computer simulations. Such astrophysical jets can be either supersonic or relativistic, and are believed to originate from accretion disks around supermassive black holes in the cores of active galactic nuclei (AGNs). During FY16, one of our specific objectives was to expand a series of large-scale, three-dimensional, relativistic hydrodynamic simulations of jet propagation into the relativistic, magneto-hydrodynamic range. We explored the parameter space for these jets in order to gain a more complete understanding of the modes of jet-ambient-medium interaction. This effort enables NRL to engage in state-of-the-art three-dimensional relativistic hydrodynamic and magneto-hydrodynamic modeling.

Methodology: The work consists of developing and running large-scale multidimensional simulations with the PLUTO code, which has the capability of simulating hydrodynamic (HD), magnetohydrodynamic (MHD), and relativistic, magneto-hydrodynamic (RMHD) processes. For the HO regime, we have used the VH-1 code (an older, three-dimensional (3D) piece-wise parallel numerical hydrodynamics code), which we ported to the NRL HPC SGI Altix machines, in order to benchmark the PLUTO code. We are continuing to explore the jet evolution in the relativistic, and RMHD regimes. We have explored the effects of gravity gradients generated by the accretion disk that generates the astrophysical jet in order to model the jet-disk feedback mechanisms that can affect jet-launch. We also plan to incorporate plasma processes into the jet energy and momentum loss for the jet propagation in order to provide a more realistic simulation of the jet-ambient-medium interaction by incorporating these "microscopic" processes. The resulting plasma-incorporated simulations can then provide a self-consistent estimation of the expected radiation in the form of both thermal radiation and synchrotron emission.

Results: We have ported, compiled, and run highly parallelized versions of both the PLUTO and the VH-1 codes for the largest simulation thus far (1024^3 cells). Smaller benchmarking simulations (512^3 cells) allow us to investigate the jet velocity parameter space to determine how it affects the development of jet-induced turbulence in the ambient medium. We have simulated jet velocities of 0.5c to .998c, where c is the velocity of light, utilizing the RMHD regime with the PLUTO code. Figure 1 shows the fully 3D RMHD simulation of gas density structures of an astrophysical jet seen in cross-section at a time of 4.0×10^7 years, a bulk velocity of v=0.995c. The jet initially has a magnetic field of order micro-Gauss for both poloidal and toroidal components. Note the well-developed Rayleigh-Taylor instabilities at the jet-ambient medium boundary despite the presence of the magnetic field. The simulation size is ~64 kpc on a side and we show the structure after $\sim 10^4$ time steps. In this simulation, the jet-to-ambient medium density ratio is 1/100 and the ratio of jet input pressure to ambient medium pressure is 5×10^{-3}.

DoD Impact/Significance: Many U.S. Government agencies, in addition to the DoD, have an interest in developing a robust capability to model hydrodynamically plasma and fluid systems in a highly anisotropic medium. A related and closely following interest is in developing the ability to model radiative transfer in such a multi-dimensional plasma and fluid environment. These calculations will advance the science of modeling astrophysical and near-earth space plasma environments.

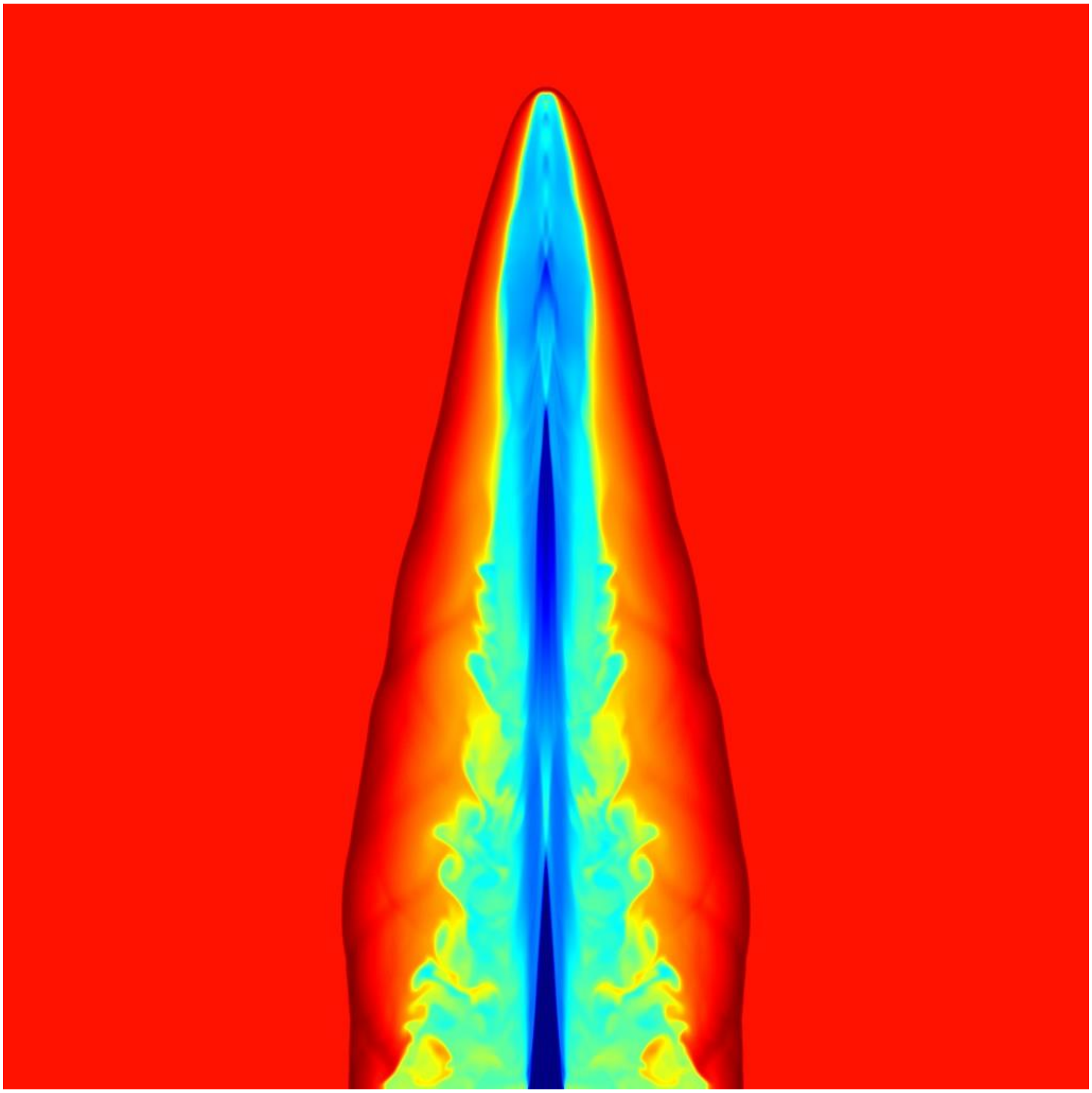


Figure 1. 3D simulation of an astrophysical jet gas density structures seen in cross-section at a time of $4.0x10^7$ years, for a bulk velocity of v=0.995c. This simulation utilizes 512^3 grid cells. Note the well developed Rayleigh-Taylor instabilities at the jet-ambient medium boundary. The simulation size is ~512 kpc on a side and we show the structure after $\sim 10^4$ time steps. In this simulation, the jet-to ambient medium density ratio is 1/100 and the ratio of jet input pressure to ambient medium pressure is $5x10^{-3}$.

Title: A Large N-Body Simulation Testing High-Velocity Galaxy Cluster Mergers
Author(s): E. Polisensky
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: SAS

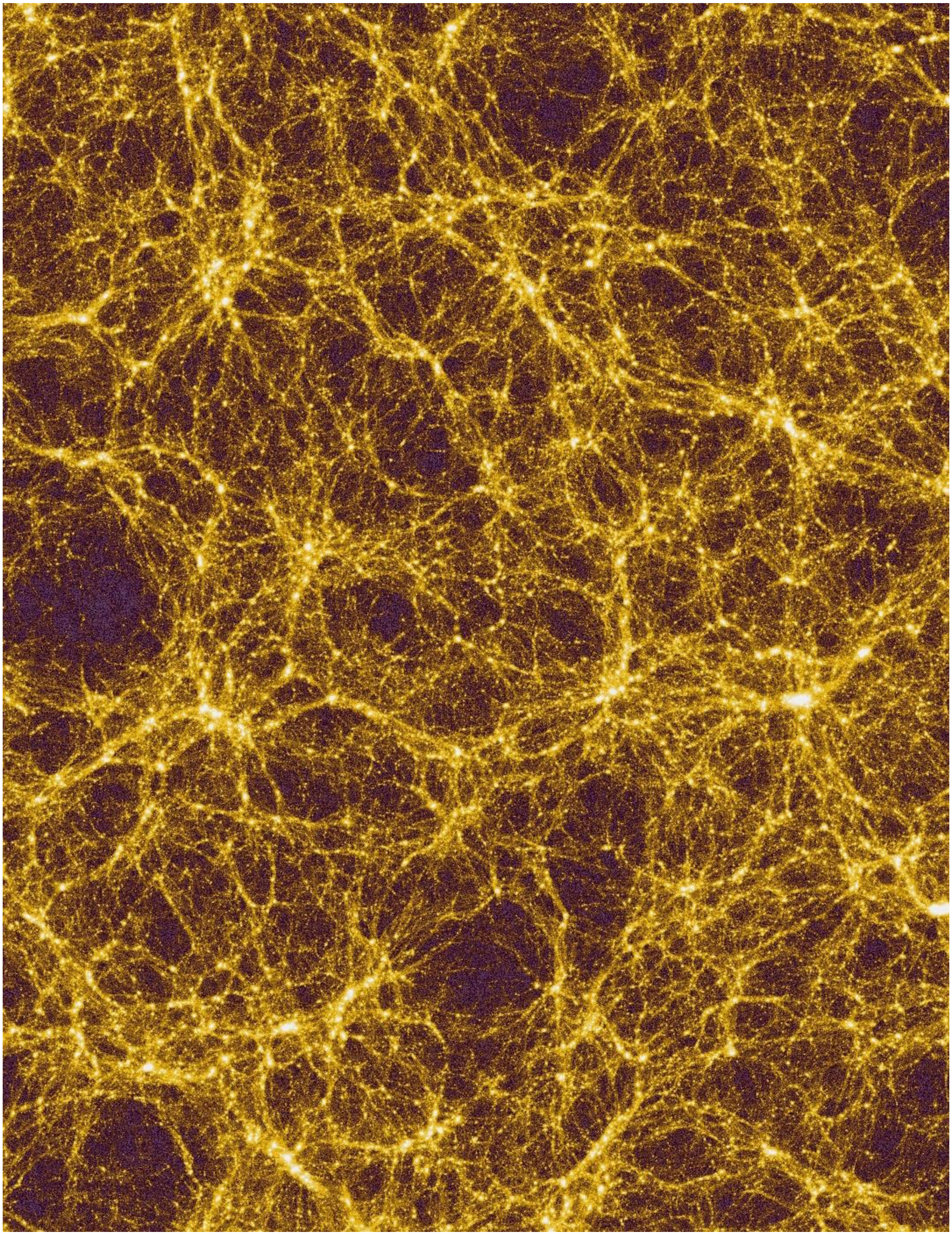
Computer Resources: SGI ICE X [AFRL, OH]

Research Objectives: Optical, radio, and X-ray observations have revealed merger velocities in excess of 3000 km/s in the massive galaxy clusters 1E0657-56, MACS J0717.5+3745, El Gordo, and Abell2443. These large velocities have been argued to be inconsistent with simulations of cosmic structure formation in the standard model of a universe dominated by dark matter and dark energy. State of the art simulations sample extremely large volumes but are limited by low mass and time resolutions and in their ability to identify merging halos at small separations where the largest velocities are observed. The objectives of this HPC project were to conduct simulations with high time resolution to track merging halos throughout their orbits and probe the velocities at distances less than one million light years.

Methodology: Achievement of our objectives faced several challenges. Several billion particles were required to achieve the necessary mass resolution in a statistically significant volume. To achieve the necessary time resolution required 20,000 integration steps and 100 TB of scratch space to store the raw particle data at hundreds of times. We also required an N-body code scalable to thousands of processing cores. To meet these challenges, we obtained the parallel code GADGET3 to numerically evolve the dark matter gas using tree and particle mesh algorithms to calculate the gravitational forces from initial conditions generated with second order Lagrangian perturbation theory with the MUSIC software. We performed a series of small scale trials to find the optimum set of GADGET3 parameters defining the size of the integration steps, scale between long-range and short-range gravitational force calculations, and run time to meet our computational requirements.

Results: With our efficient parameter set we were able to run simulations with 5 billion particles across three cosmological volumes allowing us to meet our goals of high time and mass resolutions and also to sample large volumes for statistically rare merging systems. A projection of the three-dimensional density field showing many large galaxy clusters in a small volume of our simulations is shown in the accompanying Figure. Our final data set consisted of mass, position, and velocity data for approximately 4,000,000 halos at nearly 500 times across 10 billion years. The computational challenges of constructing merger trees for such a large data volume are great and will be the focus of work in the coming year.

DoD Impact/Significance: Mergers between massive galaxy clusters are the most energetic events in the universe, and are unique laboratories for studying the physics of plasmas interacting with magnetic fields at high temperatures and low densities. The growth rate and abundances of galaxy clusters are sensitive to the fundamental matter and energy components of the universe and their gravitational dynamics are dominated by dark matter of unknown composition. Dark matter cannot be detected by direct observation but can be modeled with HPC techniques. Understanding galaxy clusters can potentially lead to breakthroughs in fundamental physics which can lead to new funding opportunities and new technologies. The computational techniques developed in this basic research program will additionally be applicable to future basic and applied NRL projects including computer-intensive real-time ionospheric monitoring with the NRL NRAO VHF systems and pulsar detection with NRL's Long Wavelength Array.



Simulation of the matter density of the Cosmic Web at the present time. Galaxy clusters are located in region of high density (white). The image is approximately 2 billion light-years across.

Title: Dynamic Phenomena in the Solar Atmosphere
Author(s): M.G. Linton
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: SAS

Computer Resources: Cray XE6, Cray XE6m [ERDC, MS]; Cray XC30, SGI ICE X [AFRL, OH]; Cray XC40 [ARL, MD]

Research Objectives: The goal of this HPC program is to understand and to model the solar drivers of the violent space weather that disrupts DoD and civilian communications, navigation and surveillance systems. The program is focused on understanding, and ultimately predicting, the initiation processes of the two key solar drivers: coronal mass ejections (CMEs) and solar flares. The fundamental questions that we are investigating with our numerical simulations are how flux emergence and photospheric twisting or shearing drive CMEs and flares, and how the reconnection which releases energy in these events occurs in both coronal and chromospheric conditions.

Methodology: We are concentrating our efforts on studying how flux emergence and photospheric driving energizes the chromosphere and corona, and how this in turn drives solar activity. During the past year we focused on investigations of the propagation of magnetoacoustic waves up from the photosphere into the overlying atmosphere, and on the processes, which deflect and dissipate these waves in the chromosphere and corona. In parallel, we focused on development and testing of photospheric data driving methods for driving our atmospheric simulations from observations, and on larger scale flux emergence and CME eruption simulations. For these studies, we used our state-of-the-art magnetohydrodynamical Lagrangian remap code LAREXD for two-dimensional (2D) and three-dimensional (3D) simulations.

Results: We have simulated the propagation of magnetoacoustic waves, excited in the photosphere, as they propagate up through the chromosphere and corona. We have investigated how the associated wave energy is transferred from one mode to others, and how the energy is deflected by magnetic topological features in the simulation and converted to heat at current sheets. This work is giving key insights into how these waves could generate observable emission signatures in the chromosphere and photosphere. We have developed and tested numerical methods for driving the solar atmospheric evolution from observed photospheric magnetic field evolution. We have tested this method on synthetic photospheric data derived from our flux emergence simulations, and have shown that under idealized conditions, the method produces an atmospheric evolution with vanishingly small errors. When the boundary is driven with more realistic data representative of observational capabilities, the errors increase, but remain reasonable for features, which evolve slowly relative to the driving cadence. In parallel with this work, we have extended our 3D studies of magnetic flux emergence to realistic solar active region time and spatial scales. From these results, we have found that active region sized flux emergence can produce breakout CME eruptions in conditions comparable to those we found at smaller scales. We have also found that the emergence time of these regions increases with their magnetic flux, following the observed behavior of similar regions.

DoD Impact/Significance: These numerical simulations are providing new insight into how photospheric flux emergence and wave driving energize the chromosphere and corona. The results show both that magnetic flux emergence is an important means of creating complex coronal magnetic structures, and that these structures can be recreated in simulations via accurate boundary driving of the photosphere. Furthering this understanding will form a fundamental step forward in building space weather prediction models, and toward avoiding some of the damaging effects of space weather.

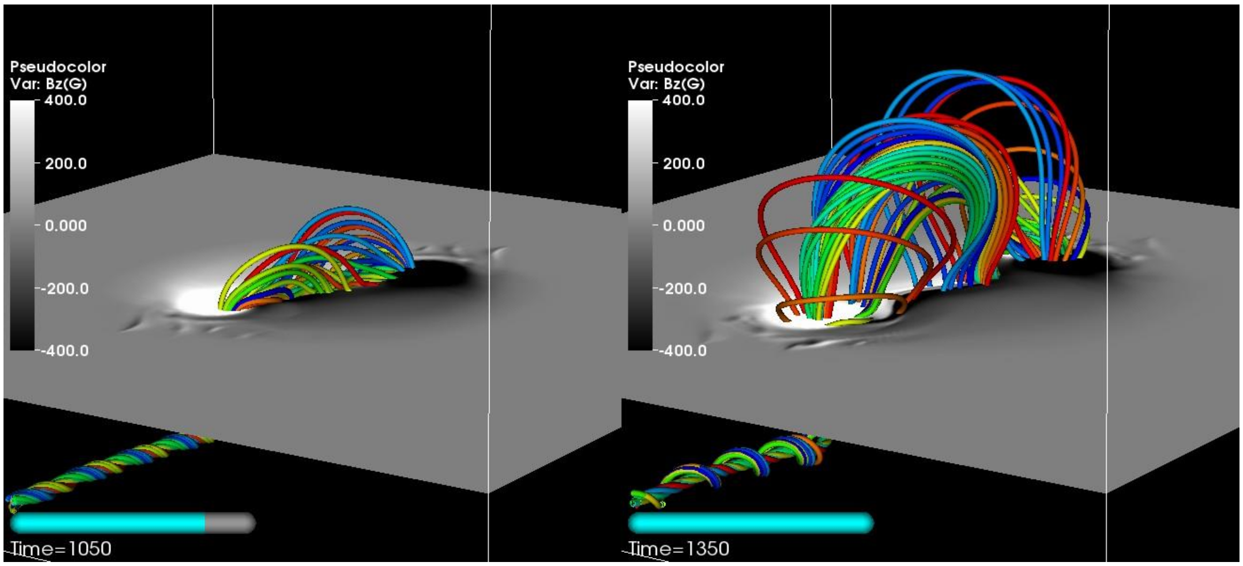


Figure 1. This figure illustrates the formation of a magnetic active region with a sheared arcade during the simulated emergence of a magnetic flux rope from the convection zone up into the solar atmosphere. The gray-scale surface shows the vertical magnetic field at the solar photosphere. The colored lines follow the magnetic field lines. The final footpoint separation of the emerged active region is 70 Mm, and its magnetic flux is 10^{22} Mx. Both are comparable to that of a medium sized solar active region.

Title: Development of a Weather Model of the Ionosphere
Author(s): S.E. McDonald,[1] D.P. Drob,[1] D. Siskind,[1] and J. Tate[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]Computational Physics, Inc., Springfield, VA
CTA: SAS

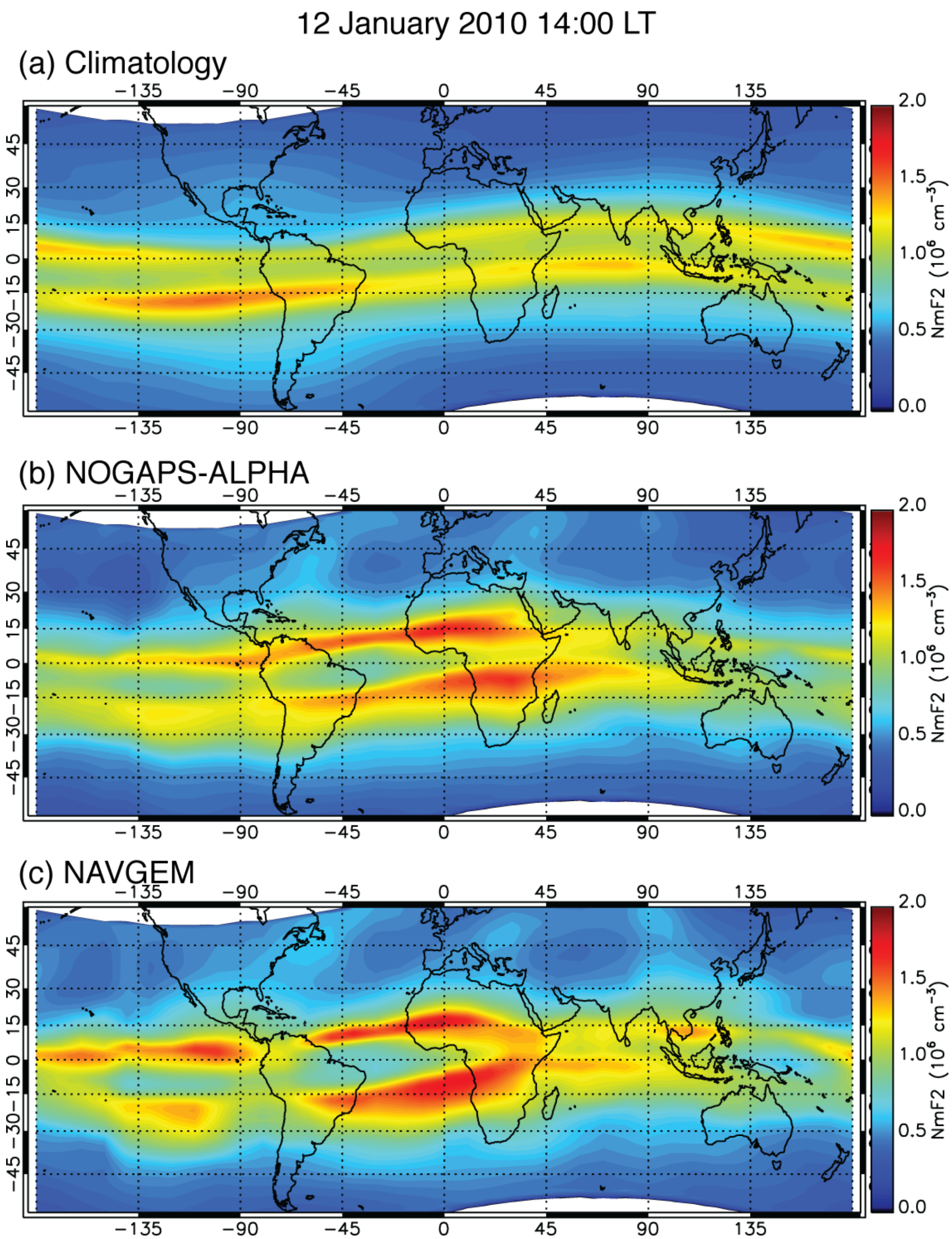
Computer Resources: SGI ICE X, Cray XC30 [AFRL, OH], IBM iDataPlex [NAVY, MS]

Research Objectives: The scientific goal of the proposed research is to characterize and simulate the physical processes that are important for improving numerical forecasting of high-frequency (HF) radio wave propagation through the Earth's atmosphere and ionosphere across the range of conditions relevant to DoD operations. In FY16, the main objectives were to conduct tests of SAMI3 and WACCM-X as we develop a fully coupled atmosphere-ionosphere model, validate the ionospheric output, and investigate lower atmospheric effects on the ionosphere.

Methodology: We are developing the Highly Integrated Thermosphere and Ionosphere Demonstration System (HITIDES), which consists of SAMI3, a state-of-the-art NRL model of the ionosphere, along with couplers that use the Earth System Modeling Framework (ESMF) for interpolation between the atmosphere and ionosphere grids. HITIDES is currently being integrated with the Whole Atmosphere Community Climate Model eXtended (WACCM-X) but is being designed to work with any NUOPC (National Unified Operational Prediction Capability) and ESMF compliant whole atmosphere model that includes a thermosphere. In FY16, we continued to optimize SAMI3 and improve memory management. Numerous tests were performed to ensure interpolation from the WACCM-X grid to the SAMI3 grid was not introducing significant errors into the results. We also performed simulations of January 2010 using meteorological forcing from NOGAPS-Alpha and NAVGEM.

Results: In FY16, we completed the one-way coupling of SAMI3 to WACCM-X. SAMI3 now runs within the WACCM-X 5-minute time-step, using the WACCM-X winds, temperatures and neutral densities. The WACCM-X output is interpolated from a regular grid onto the SAMI grid at each timestep; the values are also extended in altitude from the top of the WACCM-X grid (~500 km) to the top of the SAMI grid (~20,000 km), using spherical harmonics. Previously we have investigated the impacts of thermospheric winds on ionospheric electron densities, including effects from meteorology by constraining WACCM-X with 6-hour data products from NOGAPS-Alpha. In FY16, we have begun to investigate the effects of the neutral densities and temperatures. Inclusion of the WACCM-X thermospheric constituents has improved the simulation of day-to-day variability of the bottomside ionosphere. Additionally, we have performed runs with forcing from the 3-hour NAVGEM products for the month of January 2010 and compared the simulations to runs using the 6-hour NOGAPS-Alpha products. NAVGEM can better resolve semi-diurnal tides in the atmosphere and initial analysis of the HITIDES simulations show that this leads to significant improvements in the specification of the ionospheric densities. Our work has also revealed areas in need of improvement in the WACCM-X thermospheric densities. We have continued to work on optimization of SAMI3. Improvements in the usage of MPI in the code along with better memory management have contributed to a faster code.

DoD Impact/Significance: This effort will lead to a better understanding of the physics, dynamics, and chemistry of the bottomside ionosphere, with direct implications on future capabilities for nowcasting and forecasting of the environment relevant to DoD/Navy systems.



Navy-HITIDES simulations of peak electron density (NmF2) shown at a constant local time of 14:00 LT on 12 January 2010 using (a) climatological thermosphere from HWM14 and NRLMSIS, (b) thermosphere from WACCM-X forced with 6-hour NOGAPS-ALPHA data products and (c) thermosphere from WACCM-X forced with 3-hour NAVGEM data products. The climatological thermosphere yields very little longitudinal structure, whereas the simulation using NAVGEM shows considerable ionospheric structure resembling observations.

Title: Radio and Gamma-Ray Searches for Millisecond Pulsars and Radio Transients*
Author(s): P.S. Ray and J. Deneva
Affiliation(s): Naval Research Laboratory, Washington, DC
CTA: SAS

Computer Resources: SGI Altix ICE [NRL, DC]

Research Objectives: The purpose of this project is to search for millisecond pulsars in gamma-ray data from NASA's Fermi Large Area Telescope as well as pulsars and radio transients in ground based data from the Robert C. Byrd Green Bank Telescope in West Virginia and the Arecibo telescope in Puerto Rico. These searches require high performance computing resources because of the massive parameter spaces that must be searched.

Methodology: We use custom codes to search for pulsations in our radio and gamma-ray data sets. These correct for frequency-dependent delays caused by interstellar dispersion and variable Doppler shifts caused by orbital acceleration in a binary system then search over a broad range of candidate frequencies using very large Fourier transforms and harmonic summing. We split up the trials over a set of nodes on the cluster.

Results: During FY16 we searched 264 hours of data from the 327 MHz Arecibo drift pulsar survey (AO327). This survey began in 2010 and aims to cover the part of the sky accessible to the Arecibo telescope by 2017. It is currently the largest conducted with the Arecibo telescope, both in terms of sky coverage and observing time allocation. NRL was one of three processing sites this year, in addition to the University of Texas at Brownsville and the University of New Mexico. Our code for automatically selecting radio transient candidates based on their likelihood of originating from an astrophysical source discovered 3 new objects: 1 pulsar and 2 rotating ratio transients. In addition, students looking through candidates from our periodicity search found 5 new pulsars, including 3 millisecond pulsars in binary systems. The position uncertainty of one of these 3 pulsars overlaps with the error ellipse of a Fermi unidentified gamma-ray source. We are carrying out additional observations with Arecibo to determine the pulsar's position more precisely and confirm or rule out association with the gamma-ray source.

We also searched 195 hours of Arecibo data at 327 MHz and 1400 MHz from a deep search for radio pulsations in 14 Fermi unidentified sources. This project resulted in the discovery of one binary millisecond pulsar that is a promising candidate source for Pulsar Timing Arrays (PTAs).

DoD Impact/Significance: The main goal of AO327 is to find millisecond pulsars that are very stable rotators and therefore useful for detecting gravitational waves with a Pulsar Timing Array. Among the ~2300 known pulsars, only 35 fit this criterion and any addition to this set is a significant contribution to the gravitational wave detection effort as it improves the sensitivity of the PTA. To date, AO327 has contributed two such discoveries to the PTA. Another major goal of the survey is to catalog the local pulsar population at 327 MHz, which would contribute to improved models of the pulsar population and evolution in the Galaxy as a whole.

Our searches are part of a worldwide campaign to understand the nature of the large population of unidentified gamma-ray sources being uncovered by Fermi. The large population of millisecond pulsars in short-period interacting binaries (the black widows and redbacks) has been a real surprise. This work is an important contribution to the science return of the major NASA mission and will help us understand the physics and astrophysics of neutron stars, one of the most extreme environments anywhere in the universe.

*This work was supported by NASA.

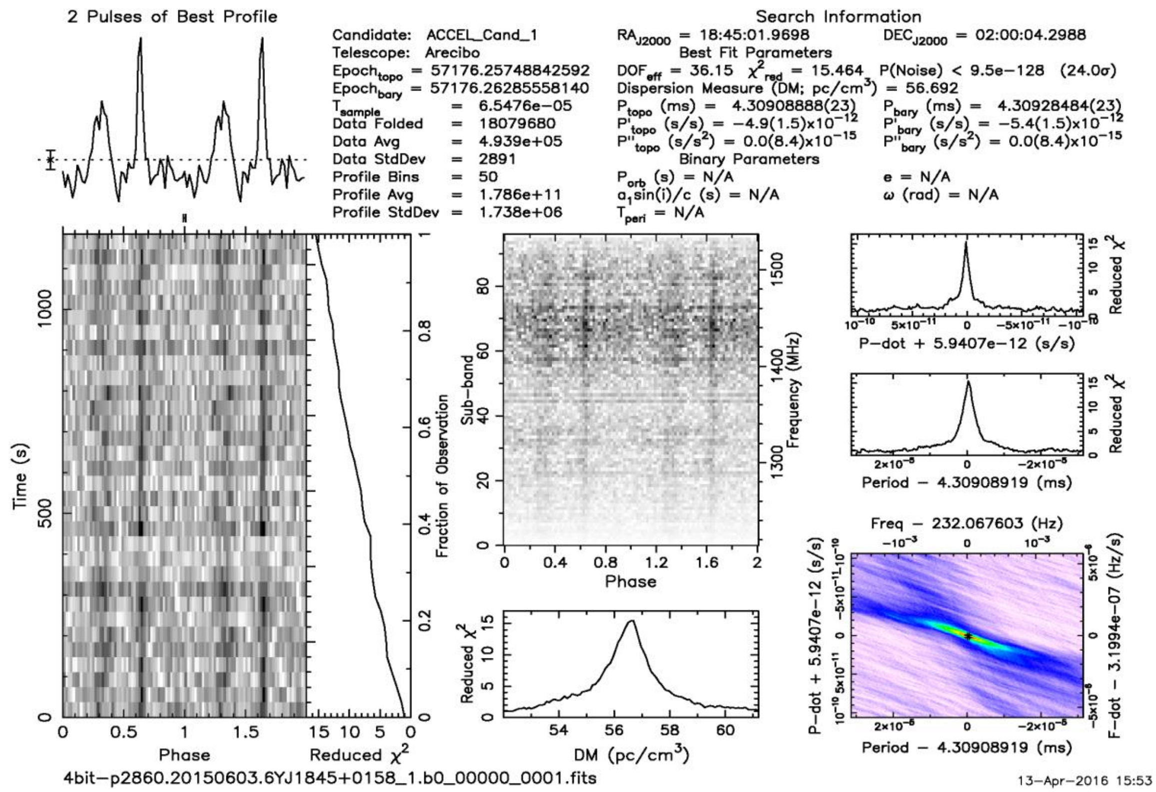


Figure 1. Discovery of the millisecond pulsar J1845+02 in our Arecibo search for radio pulsars in Fermi unidentified sources. This pulsar has a rotation period of 4.3 ms and is in a binary system with a 5.3-day orbital period. The companion star is a white dwarf. The pulsar's brightness and narrowly peaked pulse profile make it a good candidate for inclusion in Pulsar Timing Arrays with the goal of detecting gravitational waves.

Title: Meteorology and Climatology of the Thermosphere
Author(s): D.P. Drob,[1] J.T. Emmert,[1] and M. Jones[2]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]National Research Council Post Doctorial Program, Washington, DC
CTA: SAS

Computer Resources: SGI ICE X [AFRL, OH]

Research Objectives: This effort seeks to gain new insights into the coupled geophysical processes governing the meteorology and climatology of Earth's thermosphere. This requires a detailed accounting of the mass, momentum, and energy budgets of the thermosphere as perturbed from below by tides, planetary waves, and sub-grid scale fluctuations; as well as from above by Extreme Ultraviolet (EUV) flux and solar wind driven magnetic field fluctuations.

Methodology: NRL is upgrading its widely used empirical models MSIS® (Mass Spectrometer and Incoherent Scatter) and HWM (Horizontal Wind Model). These provide observationally driven specifications of the state variables of the thermosphere as a function of day-of-year, latitude, longitude, local time, solar flux, and geomagnetic activity. These upgrades involve the optimal estimation of 2×10^4 multivariate non-linear model parameters from a diverse forty-year historical database of satellite- and ground-based upper atmospheric observations. To provide a priori physical constraints in data sparse regions and develop new geophysical insights this effort also makes use of numerical experiments from physics-based first-principles upper atmospheric general circulation models. The National Center for Atmospheric Research (NCAR), Thermosphere Ionosphere Mesosphere Electrodynamics General Circulation Model (TIME-GCM) and the Thermosphere Ionosphere Electrodynamics General Circulation Model (TIE-GCM) are run to provide the necessary time dependent accounting of the mass, momentum, and energy budgets of the neutral upper atmosphere given corresponding specifications of the observed external system drivers from above and below.

Results: Preliminary numerical experiments were performed with the TIME-GCM to evaluate how different lower atmospheric drivers effect the climatological semiannual oscillation in globally-averaged thermospheric mass density. This semiannual oscillation is the second largest seasonal variation of the global thermospheric total mass density resulting in a 25% density change in global average total mass density at 400 km over ~90 days. Although the thermospheric semiannual oscillation was discovered over 40 years ago, its occurrence presently does not have a universally excepted theoretical explanation. Our results show that the TIME-GCM is capable of simulating from first-principles the semiannual oscillation in globally-averaged mass density, including a related variation in global ionospheric total electron content electron, with the amplitude and phase comparing well with observations. Through diagnosis of the globally-averaged continuity equation for atomic oxygen, our results show that the upper thermospheric semiannual oscillation originates in the mesopause, where a semiannual oscillation in atomic oxygen is forced by seasonal variations in the diffusive, advective, and net tidal transport of atomic oxygen.

DoD Impact/Significance: The specification of thermospheric neutral density, composition, and wind is the largest source of uncertainty for predicting the future position of low earth orbiting objects for collision avoidance and orbital decay applications. The specification of atomic oxygen densities is also very important for space mission operations, planning and design, as reaction with the corrosive atomic oxygen atoms erode many materials, including a number of polymers, mirror coatings, and spacecraft components. The neutral thermosphere is also the primary drivers of the day-to-day variability of the ionosphere, the understanding of which is vital to the optimal operation of DoD High Frequency (HF) RADAR and communication systems.

ENS

Electronics, Networking, and Systems/C4I

ENS focuses on the use of computational science in support of analysis, design, modeling, and simulation of electronics from the most basic fundamental, first principles physical level to its use for communications, sensing, and information systems engineering. Accordingly, ENS activity ranges from the analysis and design of nano-devices to Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR) systems-of-systems. This focus ties together nano-electronics, acousto-electronics, micro-electro-mechanics, optoelectronics, photonics, circuits, and networks through the exploration of passive/active devices, detectors, emitters, and their physical integration and system deployment in a network-centric warfare environment. ENS methodologies have been developed to explore the nano-scale and below (e.g., electronic structure, charge transport, optical, and photonic interactions) as well as at the analog/digital circuit and communications, sensor and system level (e.g., data links and transport including signal propagation) for performance analysis of information warfare systems-of-systems and large tactical networks.

Title: Numerical Studies of Semiconductor Nanostructures
Author(s): T. L. Reinecke,[1] L. Lindsay,[2] and P. Dev[3]
Affiliation(s): [1]Naval Research Laboratory, Washington, DC; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Howard University, Washington, DC
CTA: ENS

Computer Resources: SGI Altix ICE [NRL, DC]; Cray XE6, Cray XE6m [ERDC, MS]; Cray XC30, SGI ICE X [AFRL, OH]

Research Objectives: To calculate the structures and the electronic properties of carbon based nanomaterials with adsorbate atoms and molecules, to guide work on chemical functionalizations, of these materials and to advance their use as chemical sensors and in advanced electronics. To make first principles calculations of the thermal conductivities of semiconductors as a basis for identifying high thermal conductivity materials for cooling in electronics. To calculate the electronic and optical properties of solid state quantum bit systems to advance their implementations in quantum information technology.

Methodology: *Ab initio* density functional calculations are made of the structural and electronic properties of carbon based nanostructure systems with chemical functionalization. *Ab initio* density functional methods are used to calculate the phonon frequencies and wavefunctions and the interactions between phonons in semiconductors and in semiconductor nanostructures, and inelastic Boltzmann equation methods are used to calculate their thermal conductivities. Electronic calculations are typically made using QuantumEspresso codes. The properties of excitations in quantum dots and other solid state systems in quantum information technology are calculated using density functional theory, finite element techniques, and the diagonalization of large matrices for many-body and optical properties.

Results:
1. Chemical functionalization of graphene is of interest for changing its properties such as band gaps and doping for use in technologies. Density functional calculations have been made for a range of adsorbates, including H, F, N, NH_2, and of their complexes with other defects. Binding energies, structures, band gaps, interactions between adsorbates and magnetic properties were calculated, and a range of physical behaviors were found.

2. Carbon based materials, including diamond and graphene, have among the highest thermal conductivities known. A rigorous first principles treatment of thermal transport in graphene has been developed using density functional techniques for phonons and their interactions and an exact Boltzmann-Peierls equation approach is used for thermal transport. Results agree well with available experiment, make predictions the effects of substrates, and show the key role played by vibrations perpendicular to the graphene layer.

3. Quantum information has opened key new opportunities in range of new technologies, including quantum sensing. Here a new approach to quantum sensing has been developed based on the optical properties of the unique spin 3/2 multiplet of a Si vacancy in 4H-SiC. The full optical properties of this defect have been calculated, and protocols for sensing of magnetic fields, strain and temperature have been developed. Sensitivities and spatial resolution beyond any currently available have been predicted.

DoD Impact/Significance: Understanding chemical functionalization of graphene and other monolayer systems will open opportunities to control their properties for use in electronics and as chemical and biological sensors. Understanding thermal conductivities in semiconductor materials and systems will make possible their exploitation in cooling and in thermoelectrics. Understanding the role of interactions and couplings between quantum bits in a range of systems will open opportunities to develop fast optical quantum computation based on them.

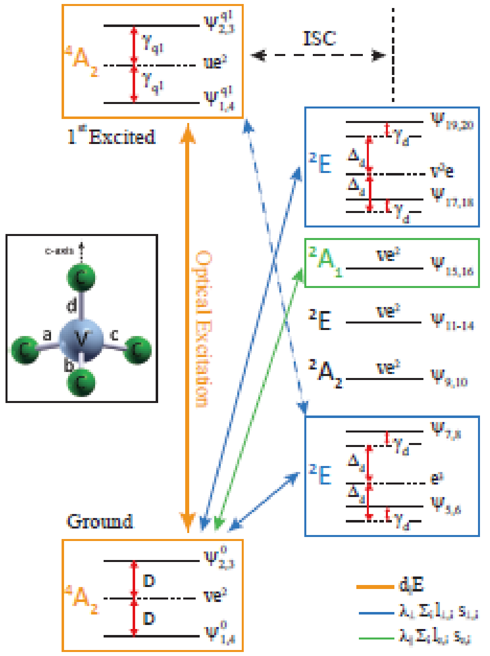


Figure 1. Electronic and optical properties of the Si vacancy defect in 4H-SiC as a basis for quantum sensing.

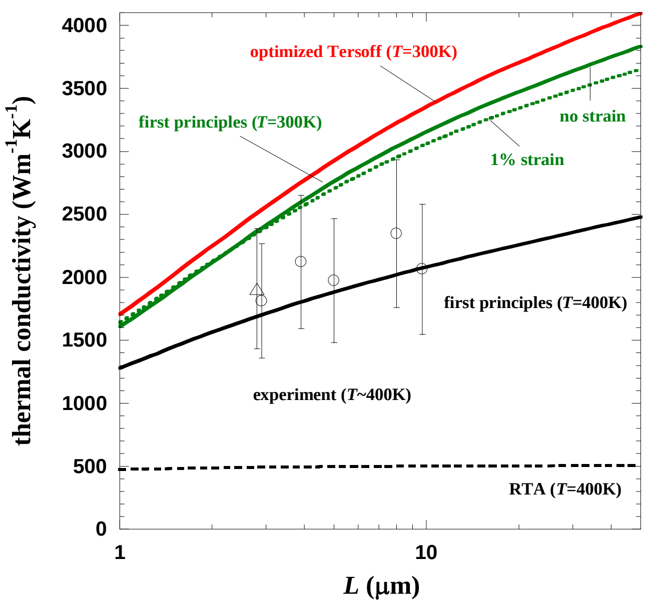


Figure 2. Calculated thermal conductivity of graphene versus sample length.

Title: Automated Translation of Hierarchical Task Network Planning to Classical Planning
Author(s): R. Alford[1] and D.W. Aha[2]
Affiliation(s): [1]ASEE Postdoctoral Fellow, Naval Research Laboratory, Washington, DC; [2]Naval Research Laboratory, Washington, DC
CTA: ENS

Computer Resources: SGI Altix ICE [NRL, DC]

Research Objectives: We sought to show that effective heuristics for hierarchical planning problems can be automatically derived by translating them into flat planning problems and using classical heuristic-search planners.

Methodology: To validate whether our translation algorithm was practical, we ran two classical planners on a set of randomly generated flat problems and their translated hierarchical duals. To validate whether our algorithms found reasonable translation bounds for “natural” problems, we ran two classical planners on all feasible translation bounds of each problem in a corpus of hierarchical problems, measuring completion rates and times.

Results: On the randomly generated problems, we showed that both planners could solve the translated hierarchical problems more efficiently than their flat counterparts. On the corpus problems, we showed that the classical planners could solve most of the translated hierarchical problems with the automatically-found upper translation bound, and that many of the remaining problems could be solved with the automatically-found lower translation bound. Taken together, our results show that translation to flat planning is an effective approach to solving hierarchical problems.

DoD Impact/Significance: The Navy needs mid- to long-range automated planning to facilitate unmanned agents in a number of environments, from aerial combat to underwater, to virtual environments for pilot training. Hierarchical planning has been used in these situations, however current hierarchical planners use blind search and rely on the domain engineer to create planning operators that limit the search in ways that a solution is quickly found. Our work shows how to automatically provide heuristic search for many hierarchical problems.

OTH

Other

Work that is not easily categorized as one of the other computational technology areas.

Title: Simulation of High-Energy Radiation Environments
Author: M. Strickman and J. Finke
Affiliation: Naval Research Laboratory, Washington, DC
CTA: OTH

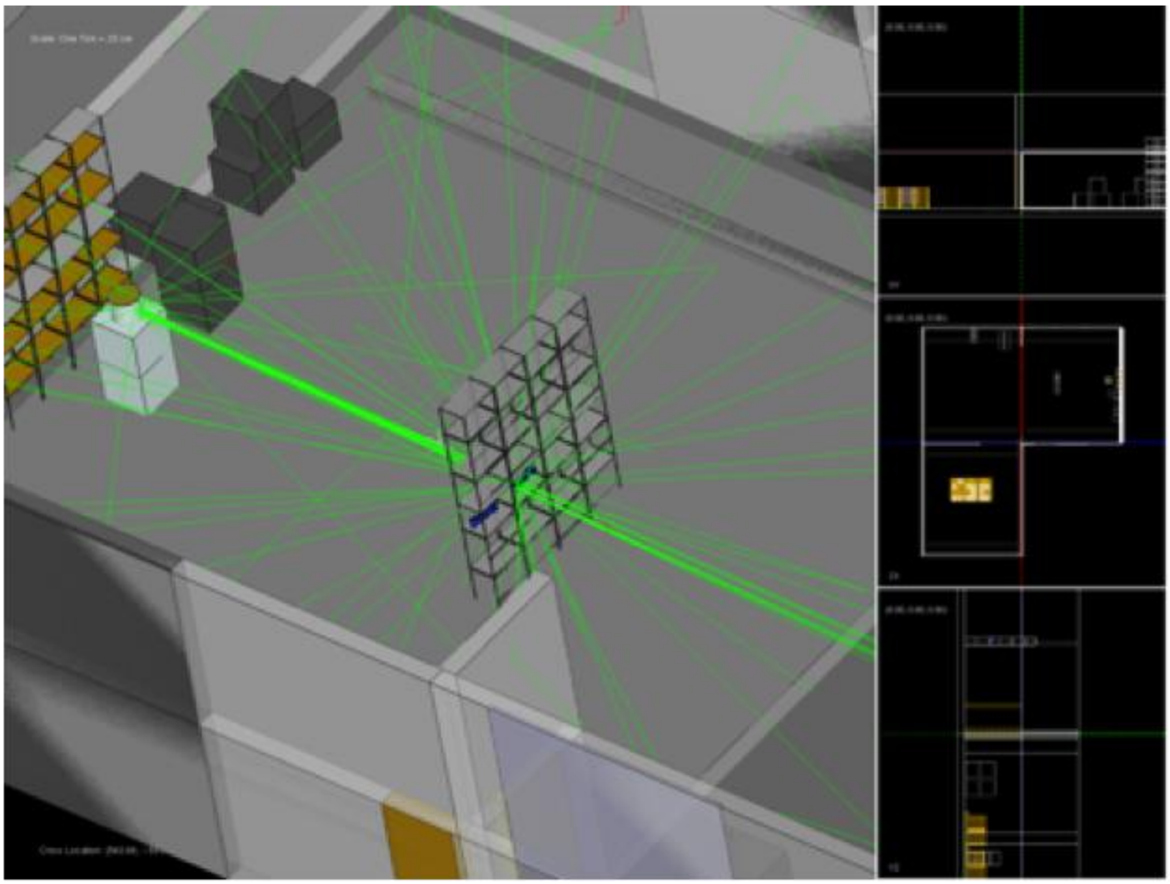
Computer Resources: SGI Altix ICE [NRL, DC]; SGI ICE X [AFRL, OH]; Cray XC40 [ARL, MD]; IBM iDataplex [MHPCC, HI]

Research Objectives: Apply 3-D Monte Carlo (MC) methods to simulate the transport of high-energy particles through matter for use in space applications as well as for modeling detection systems, radiation environments, and the operational concepts relevant to the detection of Special Nuclear Materials (SNM) and other radiological/nuclear materials in maritime and urban scenarios of interest to DoD and other civilian agencies.

Methodology: Our studies involve using three industry-standard ionizing radiation transport codes: two 3-D MC packages, Geant4 (CERN) and MCNP (Los Alamos National Lab), and one discrete ordinates package, Denovo (Oak Ridge National Lab). We use an NRL-developed front-end package called SoftWare for Optimization of Radiation Detectors (SWORD) to quickly prototype geometries and radiation environments for running our simulations. Although 3-D MC codes give very accurate results, they are computationally expensive. Fortunately, runs are easily parallelized. Simulation studies are often times iterative in nature, particularly when conducting a full range of sensitivity studies for instruments, and is only feasible with access to HPCMP platforms.

Results: Many of the simulations conducted were in direct support of Defense Threat Reduction Agency (DTRA) and the Domestic Nuclear Detection Office (DNDO) operational scenarios and/or exercises and were classified FOUO or higher. We have supported or are in the process of supporting simulations for the Data Mining Analysis and Modeling Cell (DMAMC) program at DNDO (see figure) and for optimizing upgrades to radiation detection capabilities on Stryker armored vehicles for SPAWAR/DTRA. Along with supporting these agencies, two additional simulations are discussed here. Using 3D MC radiation transport simulations via SWORD we have simulated propagation of gamma-rays and neutrons through the atmosphere in order to investigate both production and propagation of radiation from thunderstorm-related particle acceleration. One type of acceleration event, the Terrestrial Gamma-Ray Flash (TGF) produces brief, very bright flashes of gamma-rays that could contribute significant radiation dose to aircraft crew or passengers. Further study of these and other events will improve our ability to assess hazards posed by thunderstorm-related radiation phenomena. We have conducted research into gamma-ray “halos” around active galactic nuclei (AGN). MC calculations have allowed computation of halo size versus intergalactic magnetic field strength. Ultimately, comparison of these calculations with results from NASA Fermi Gamma Ray mission will constrain both halo production and intergalactic magnetic field strength.

DoD Impact/Significance: The ability to produce accurate predictions of radiation detection instrument effectiveness is crucial; it allows time and funding to be focused on creating the best possible design, rather than directing efforts to creating true physical prototypes. Similarly, simulation of radiation detection concepts of operation allows assessment of their effectiveness in realistic environments. The ability to provide timely answers to the questions posed by DNDO, DTRA, NASA, and other government sponsors is also important for the continued success in supporting the DoD mission. In addition, the science addressed by ionizing radiation simulations such as the studies described above is often impractical or not cost effective to study in any manner other than simulation. The results of these studies directly address our understanding of the high-energy radiation environment in which we live and operate.



Simulation of gamma rays illuminating a shelf of personal radiation detectors in support of the DNDO Tumbleweed campaign.

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Division/Branch Index

Center for Bimolecular Science and Engineering (Code 6900)

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Remote Sensing Division (Code 7200)

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Marine Geosciences Division (Code 7400)

Marine Meteorology Division (Code 7500)

Space Science Division (Code 7600)

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14. ABSTRACT

These reports summarize the accomplishments of the NRL Principal Investigators who received computer allocations on the DoD High Performance Computing Modernization Program Shared Resource Center in FY16.

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Biomechanics, Network encryption device, Constitutive modeling, Hyperelastic, Viscoelastic, Constrained optimization, Parameter estimation, Model calibration, Computational modeling

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